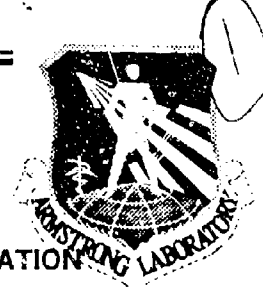


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DEVELOPMENT OF A COMPUTER-BASED AIR FORCE INSTALLATION
RESTORATION WORKSTATION FOR CONTAMINANT
MODELING AND DECISION-MAKING
USER'S MANUAL

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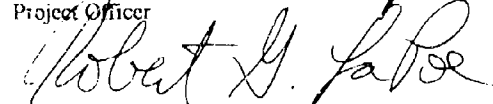
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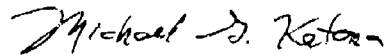
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13 ABSTRACT (Maximum of 200 words) The objective of this research is to develop a groundwater remediation advisory system for use in investigating possible remediation activities for the cleanup of contamination from hazardous substances, pollutants and contaminants at Air Force sites. The advisory system provides a decision framework for selecting an appropriate model from the numerous available transport models conditioned on available site data. In addition, the use of optimization methods is explored for determining optimal remediation strategies at a specific site. The optimization routine evaluates tradeoffs between the long-term cost of remediation and the probability the remediation strategy will fail. The final product of this project is a computer-based Air Force Installation Restoration Workstation Advisory System for contaminant modeling and decision-making. This software can be used as an aid to technical project managers within the US Air Force Installation Restoration Program in developing and evaluating possible remediation alternatives and managing ongoing remediation activities. This users manual provides guidance on use of the advisory system.		
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PREFACE

The research described in this report was conducted by Drs. Miguel A. Medina, Jr. and Timothy L. Jacobs, Department of Civil and Environmental Engineering, Box 90287, Duke University, Durham, North Carolina 27708-0287, under Contract F08635-92-C-0009, under the sponsorship of the Headquarters Air Force Engineering and Services Center, Engineering and Services Laboratory (HQ AFESC/RD), and Armstrong Laboratory Environics Directorate, Tyndall AFB, FL 32403-6001. The Project Officers were Dr. Tom Stauffer and Capt. Thomas P. deVenoge (HQ AFESC/RAVC).

This research was performed between November 15, 1991 and June 15, 1994.

Several meetings were held at Headquarters Air Force Center for Environmental Excellence (HQ AFCEE), Brooks AFB, Texas and Headquarters Air Force Engineering and Services Center (HQ AFESC), Tyndall AFB, Florida to solicit comment from potential users. After its development the software package was demonstrated to technical and administrative staff at Hill AFB, Brooks AFB, Tinker AFB and Tyndall AFB. The principal investigators wish to acknowledge the valuable suggestions received from representatives of Tinker AFB, Kelly AFB, Hill AFB, Brooks AFB, Tyndall AFB and MITRE Corporation.

EXECUTIVE SUMMARY

The objective of this research is to develop a groundwater quality modeling advisory system for use in investigating possible remediation activities for the cleanup of contamination from hazardous substances, pollutants and contaminants at Air Force sites. The application of optimization methods for determining optimal remediation (for implementation at a specific site) is also explored. This users manual provides guidance and documentation in the application of such a software package to Air Force sites. It further supplements an earlier technical report describing models and methodology, with a technical appendix describing additional models and procedures.

A 1987 Executive Order authorized the Secretary of Defense to implement the Department of Defense Installation Restoration Program (IRP). The objectives of this program include the identification, investigation, research and development, and cleanup of sites contaminated with hazardous substances from past and present activities. The Air Force has established its own in-house management and technical expertise for implementing, monitoring and managing activities within the IRP. The remedial action process consists of four discrete processes. These include: (1) Preliminary Assessment and Site Inspection, (2) Remedial Investigation and Feasibility Study, (3) Remedial Design and Remediation Action and (4) Site Closeout. The focus of the research summarized in this report impacts the implementation of the Remedial Investigation and Remedial Action phases of the remedial action process.

Over the past several decades, many different models for contaminant transport in porous media, under varying conditions and assumptions, have been proposed and tested. These range from very simple models based on one-dimensional analytical solutions, which assume a completely homogeneous and isotropic medium, to very complex models based on three-dimensional numerical solutions which allow for complete specification of the aquifer and contaminant characteristics throughout a three-dimensional grid. All contaminant transport models, regardless of the complexity of the solution method, require certain assumptions regarding the nature of the transport processes, and, therefore, can only approximate the actual spread of contaminants from a given site and the associated risks from human exposure to contaminated groundwater.

This situation presents a familiar, yet difficult problem to the analyst and the decision-makers. Sufficient data on the hydrogeology are rarely, if ever, available to apply the most complex, three-dimensional contaminant transport models to a proposed or monitored site. The analyst must choose a transport model based on a tradeoff between the presumed greater accuracy of complex models and the less onerous data requirements and easier application of simpler models. The topic of choosing an appropriate model is one of the important aspects of the advisory system developed for the Air Force, and specific algorithms have been written to assist the user with this task. These algorithms are not a substitute for first-hand experience obtained at a site.

Even with the choice of an appropriate transport model, considerable uncertainty is likely to be present in the analysis of contamination risk. Application of groundwater transport models requires estimation of parameters which are both difficult to measure and spatially variable, such as hydraulic conductivity and dispersivity. There is often good reason to doubt the accuracy of the input data. For instance, if an analytical model requires the spatial average of the hydraulic conductivity throughout the local area of the aquifer, and the available data consist of only one or two slug tests, plus perhaps an expert opinion, there is good reason to doubt that the reported best estimate of the parameter accurately reflects the true mean value. Simply running the model in a deterministic mode using the best estimates of the parameters may not provide sufficient information for a decision, because the uncertainty in the analysis has not been taken into account. For instance, if a deterministic application suggests no risk of contamination, no information is provided as to the certainty of this conclusion.

The recommended alternative is to explicitly consider the uncertainty in the analysis, through the use of techniques such as Monte Carlo analysis, Latin Hypercube Sampling, or First-Order Second Moment analysis. Uncertainty enters the modeling process in three ways: (1) through natural parameter variability; (2) through measurement error, which also introduces uncertainty in parameter estimation; and (3) through model error, representing uncertainty introduced by the degree to which the simplifying assumptions used to develop a model fail to accurately represent the actual physical processes at the site in question. The first two of these sources of uncertainty can be analyzed separately. However, the data are often insufficient: in such cases, the natural and measurement uncertainty may be combined into one source of uncertainty through the specification of the distribution of the parameter value.

The third source of uncertainty in the analysis is due to the degree to which the transport model applied may misrepresent actual processes at the site. Examples of this source of uncertainty include the sorption of contaminants to soil surfaces and degradation rate coefficients. This source of uncertainty is very difficult to quantify, and indeed may be impossible to quantify for specific sites, unless extensive sampling and monitoring data are available. The advisory system **guides** inexperienced users in the model selection process, but cannot guarantee that the user will apply the models correctly. A **caveat** is therefore appropriate: because the system is user-friendly, it may tempt users that are not qualified to understand groundwater transport models to perform an analysis and subsequently interpret the results beyond their experience level.

A Monte Carlo-type analysis, for example, requires that distributions be specified for the underlying parameters having the greatest impact on contaminant transport. Specification of a parameter distribution consists of two steps: (1) choice of a distributional form, and (2) specification of the descriptive parameters of that distribution. On the first issue, the choice of distributional form, the system does of necessity provide some limitations. That is, for models which are expected to be used in cases for which the impacted aquifer is at least moderately well-characterized, certain parameter

distributions are constrained to follow specific forms, which are generally well accepted in the literature. For instance, in some of the models the mean hydraulic conductivity must be specified by a log-normal distribution. However, even in these cases, a choice is present in the parameterization, as the mean hydraulic conductivity may be directly specified from the log-normal, or generated from underlying parameter distributions. In general, where the parameters are at least moderately well known the choice of a distributional form should not have a major impact on the results. In its present form, the Advisory System incorporates the **framework** for Monte Carlo and First Order Second Moment analysis, but additional research is needed to develop the parameter distributions and values for site-specific hydrogeologic conditions.

In addition to aiding in the choosing of an appropriate mathematical model for a specific site, the Advisory System determines efficient or optimal remediation strategies. The optimization routine evaluates tradeoffs between the long-term cost of remediation and the probability the remediation strategy will fail. A chance-constrained optimization model has been developed to determine the most efficient groundwater remediation strategies. It is multiobjective and driven by probabilistic measures of contaminant concentration in the groundwater surrounding the hazardous waste site. The chance-constrained model is used to determine the tradeoffs that exist between short-term and long-term remediation costs and the probability that the remediation strategy will fail.

The development of an efficient, effective and reliable remediation strategy requires a clear understanding of the site characteristics and the remediation actions implemented. In addition, the optimal remediation strategy must consider tradeoffs between the remediation cost and the reliability of the remediation strategy. By investigating these tradeoffs, the decision maker can more accurately assess remediation needs, feasible remediation strategies and remediation strategy effectiveness.

Long-term remediation costs depend on specific remediation considerations and actions. Examples of possible remediation strategies include pulse pumping and treatment, and continuous pumping and treatment. Potential cost savings are realized by varying the long-term remediation action. The reliability of the long-term remediation strategy represents the likelihood that contaminant concentrations within the groundwater exceed specified maximums and are modeled as constraints. Using this methodology, optimal groundwater remediation strategies are determined by minimizing the long-term and short-term costs associated with the site remediation. The optimal remediation strategies are conditioned on the probability that the contaminant concentration at any time does not exceed prespecified maxima. The actual concentrations at any specified coordinates are calculated by solving the governing differential equations for groundwater contaminant flow in which key site characteristics are expressed as random variables. The resulting optimization model is solved using a second moment formulation combined with Monte Carlo simulation. Although the results of such an optimization are based upon extensive physical data, recommendations should be confirmed with site-specific hydrogeologic investigations.

The actual advisory system introductory and help screens, prompts, menus, and tabular and graphical aids have been captured as images and (although they are displayed in color on the computer screens) are presented in the text in black and white and/or gray tones. The resolution of these images is generally superior, as displayed by the monitor screen. Nevertheless, the user should be able to follow the examples in the manual clearly, and simulate them directly with the software package; extensive data sets are provided for that purpose. The users manual for the UNIX version is also available as an integral part of the software package.

The final product of this project is a computer-based Air Force Installation Restoration Advisory System Workstation for contaminant modeling and decision making. This users manual, along with the first-year technical report, fully documents the Advisory System, for two versions running under different operating systems: either the DOS or the UNIX environments. This software can be used as an aid to technical project managers within the U.S. Air Force Installation Restoration Program in developing and evaluating possible remediation alternatives and managing ongoing remediation activities.

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SECTION I

INTRODUCTION

A. OBJECTIVES

Air Force needs for contaminant transport mathematical modeling and decision-making, in terms of the predictive requirements of the Installation Restoration Program (IRP), may at least be partially addressed by development of an interactive, user-friendly **computer-based engineering workstation**. Background information on Department of Defense environmental restoration efforts and, specifically, the Air Force IRP is presented in the next section. The principal element of the workstation is an advisory system incorporating basic software to: define the magnitude, extent, direction, and rate of movement of identified contaminants; identify significant public health and environmental hazards of migrating pollutants; recommend candidate remedial actions; maintain databases of model parameters, and accomplish other supporting tasks. The principal function of a workstation is to provide optimal and efficient support to its user regarding the tasks determined for the user/workstation entity. Generally, this function can be divided into a number of subfunctions which are determined by analyzing the tasks performed by the intended users and the hardware/software environments available. Important elements in this analysis are determining the amount and type of data and establishing the level of synthesis required to adequately perform the required tasks. Furthermore, the various levels of expertise of potential users must be determined and accommodated for in the operating system to provide users with adequate assistance. This report constitutes a **users manual** for both the MS-DOS (Microsoft Disk Operating System) version and the UNIX version of the advisory system.

B. BACKGROUND

The legal mandate for the Air Force (AF) Installation Restoration Program (IRP) is the Comprehensive Environmental Response, Compensation and Liability Act of 1980 (CERCLA, known as the Superfund Act) and the Superfund Amendments and Reauthorization Act of 1986 (SARA). Section 211 of SARA deals with the Defense Environmental Restoration Program (DERP), of which the IRP is the primary subcomponent (Reference 1). A 1987 Executive Order provided authority to the Secretary of Defense to implement the Department of Defense (DOD) Environmental Restoration Program within the overall framework of CERCLA and SARA. The objectives of the IRP include "the identification, investigation, research and development, and cleanup of contamination from hazardous substances, pollutants, and contaminants." The program is focused on cleanup of detected contamination from past activities, but as noted includes research as well as development and

demonstration of innovative and cost-effective cleanup technologies. IRP activities are managed centrally in the Office of the Secretary of Defense and are carried out by the Military Services and Defense Agencies. Under this agreement, the U.S. Air Force retains the authority and initiative for cleanup activities at its own installations.

The Air Force has established its own in-house management and technical expertise for implementing the IRP, following a decentralized approach which places emphasis and authority with the Major Air Commands (MAJCOMs) and, in turn, with the individual installations under their jurisdiction (Reference 2). Several service organizations support the implementation of the Air Force IRP: the Air Force Civil Engineering Support Agency (AFCESA, HQ at Tyndall AFB, Florida), Armstrong Laboratory Environics Directorate, Tyndall AFB, Florida, the Center for Environmental Excellence (AFCEE, Brooks AFB, San Antonio, Texas), and the AF Regional Civil Engineer offices. Additional support is provided by the Air Force Material Command (AFMC), which is responsible for the advancement and effective management of the Air Force scientific and technical resources. An Air Force Installation Restoration Management (AFIRM) Committee has also been organized to support the MAJCOMs and review remedial action plans for complex problems.

The remedial action process is a progression of steps designed to fully analyze and address site problems, grouped functionally by stages, as follows:

1. Preliminary Assessment/Site Inspection (PA/SI) Stage,
2. Remedial Investigation/Feasibility Study (RI/FS) Stage,
3. Remedial Design/Remedial Action (RD/RA) Stage,
4. Site Closeout (SC) Stage.

Figure 1 illustrates these four stages and 14 steps of the remedial action process. The opportunity for application of contaminant transport models arises primarily in the **second** (investigation) and **third** (cleanup) stages. However, mathematical models may be used in the first stage in the case of unknown subsurface sources of contamination: the most likely location of the source could be calculated from known field measurements of the edge of the plume — as part of the discovery and preliminary assessment steps.

In the second stage, mathematical models may be applied to:

- Estimate the rate and extent of contamination migration from several sources (surface and subsurface);
- Simulate current and future scenarios of contamination and potential impacts at all locations of interest;

- Evaluate the likely effectiveness of proposed alternatives for remediating the impacts of released contaminants;
- Perform risk analysis, accounting for uncertainty in predictions, to assist in selection of the best remedial strategy.

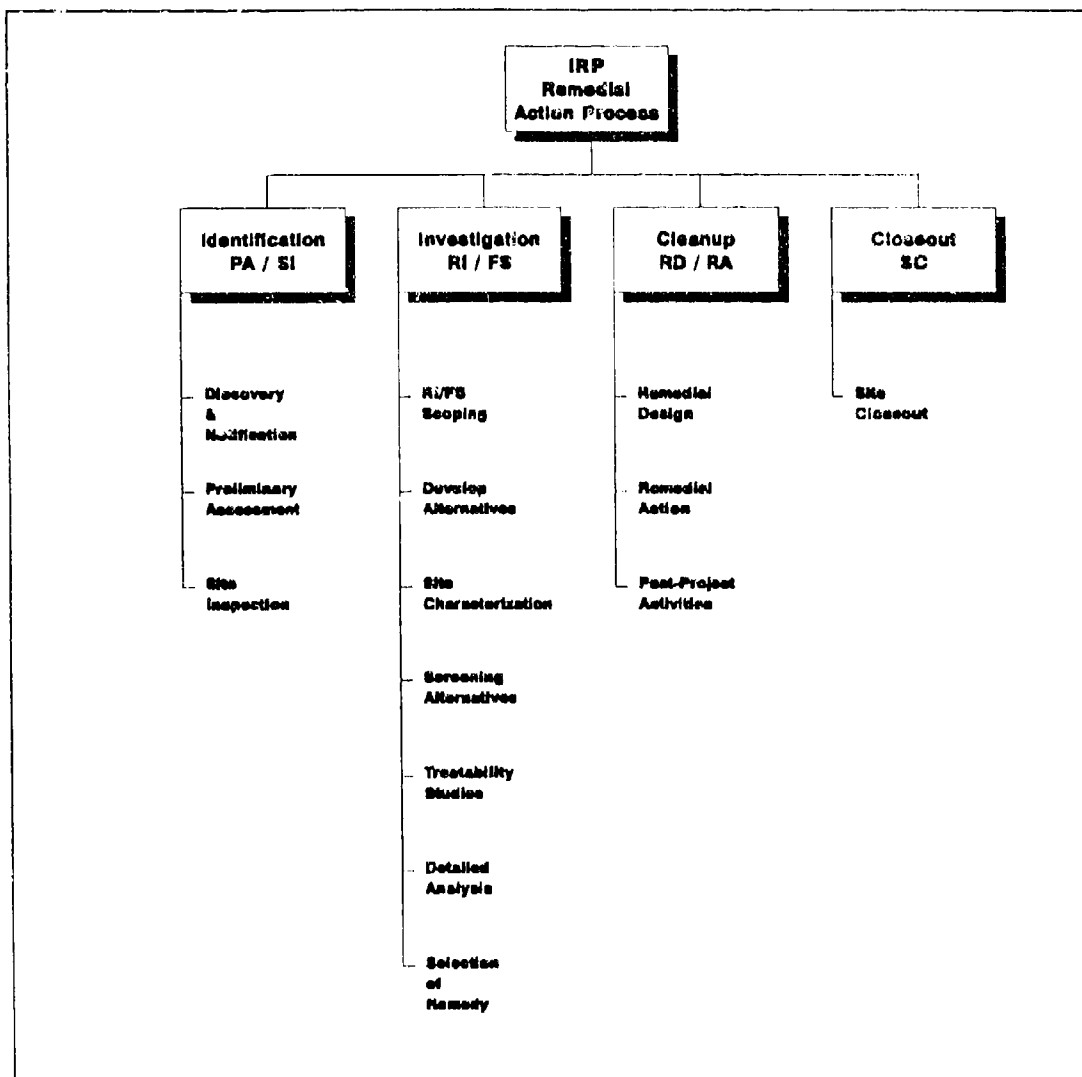


Figure 1. IRP Remedial Action Process

In the third stage (cleanup), models are useful in designing the remedial strategy: the optimal strategy should be cost-effective. Models do not reduce the need for good quality site-specific data: they help determine data needs, make better use of available data, and refine the data collection (monitoring) process to insure compliance with cleanup goals.

The Air Force Center for Environmental Excellence (AFCEE) at Brooks AFB (San Antonio, Texas) operates the technical information management system (IRPIMS) for Air Force IRP sites. It is one of the contract support centers for investigative studies. It can provide technical consultation, field monitoring, sample analysis support, and has developed programs on site ranking and Quality Assurance/Quality Control (QA/QC).

C. OVERVIEW AND COMPONENT MODELS OF THE ADVISORY SYSTEM

A flow chart illustrating the design of the workstation Advisory System is presented in Figure 2. The user/analyst interacts with a module that controls the flow between the various elements of the system. For example, to the left of the system manager are modules that access stored data (site-specific data, regional data, data on model input parameters) and preliminary screening modules (to rank the severity of contamination at the site under investigation). To the right of the manager module is a transport model selection module, named the CHOICE algorithm, discussed in greater detail below. It essentially aids the inexperienced user in selection of the solute transport model most appropriate for the site hydrogeology and method of waste disposal. After the appropriate selection is made a plume is predicted and a cumulative probability distribution of contaminant concentration is derived at any desired point in the flow field. The amount of variance in the prediction indicates the degree of uncertainty, which can be reduced by additional field sampling. The next step is optimizing the remediation process, providing a framework for evaluating remediation alternatives and implementing a solution at minimal cost and environmental risk. An algorithm to select remediation alternatives has been developed. Details of the optimization process are presented in a technical supplement (Appendix I.). If further relevant field data is available, the cycle of transport modeling begins again, to possibly reduce the variance in the predictions.

1. CHOICE, Algorithm for Model Selection

Ultimately, the management of any system means making decisions aimed at achieving the system's goals without violating specified technical and nontechnical constraints imposed on it (Reference 12). The objective function is to minimize costs and maximize the effectiveness of remediation, which can also be expressed as minimizing the probability of failure. This probability of failure may be defined as the probability of exceeding a regulatory standard.

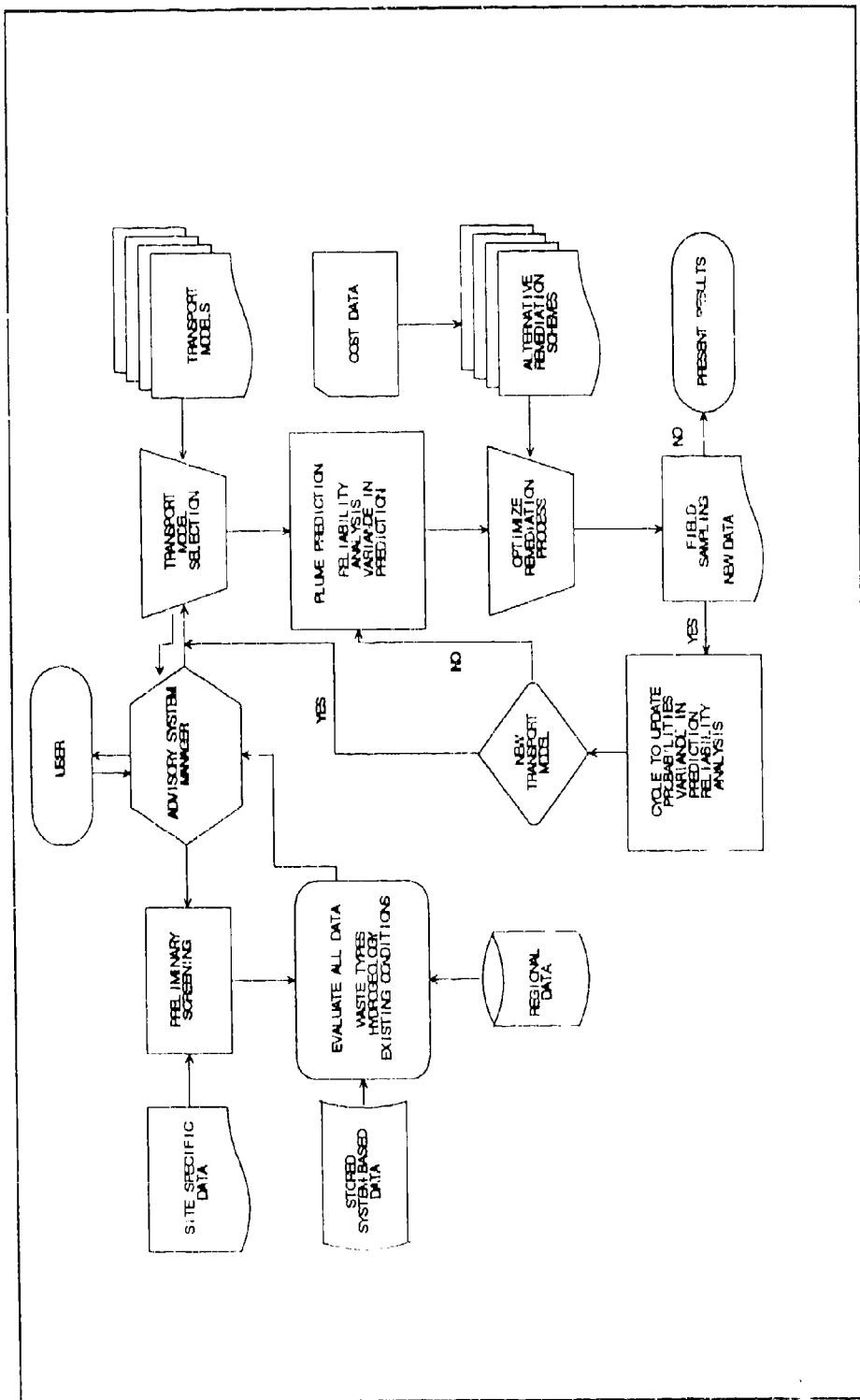


Figure 2. Workstation Advisory System Flow Chart

The nature of the overall modeling process (of which model selection is just one step) may be summarized in five general steps (Reference 13):

- **problem characterization** — the analyst clearly identifies the exposure assessment study objectives and constraints;
- **site characterization** — the analyst reviews all available data, and possibly develops a "conceptual" model;
- **model selection criteria** — the analyst matches the objective, technical and implementation criteria to available models and selects the most appropriate model(s), in this case with the aid of the CHOICE algorithm;
- **code installation** — in the case of a computer code, the model(s) should be properly installed and tested with accepted solutions to standard problems;
- **model application** — the verified model uses site data as input for the contaminant assessment.

CHOICE is not a predictive model, but rather a **screening model**. The algorithm requests information about the means of waste disposal (e.g., lagoons, landfills, rotary distributors, spray irrigation devices, etc.), the nature of the aquifer, the perimeter of compliance, penetration, type of waste and many other factors. The selection algorithm is part of an interactive, menu-driven management program which executes a large number of supporting decision algorithms and mathematical models. The mathematical details of the models are presented in the next sections, and the theoretical basis of the management modules is presented elsewhere (References 3, 5, 6, 14, and 15). Criteria for choosing among transport models have also been of regulatory interest (References 12 and 13), but without guiding the user to a specific model. The following contaminant transport models have been incorporated into the workstation advisory system:

- a. Analytical Models
 - i. One-Dimensional Transport Model, **ODAST** (Reference 16).
 - ii. Two-Dimensional Transport Model, **TDAST** (Reference 16).
 - iii. Two Dimensional Transport Model, **PLUM2D** (Reference 17).
 - iv. Two-Dimensional (x,z) Transport Model, **DUPVG** (Reference 18).
 - v. Three-Dimensional EPA Monte Carlo Transport Model **EPAGW** (Reference 19).
 - vi. EPA Monte Carlo Transport Model for Impact on Surface Waters **EPASF** (Reference 20).
 - vii. Two-Dimensional Radial Transport Model **LTIRD** (Reference 16).

- b. Semianalytical Model
 - i. Two-Dimensional Complex Velocity Potential Model, **RESSQ** (Reference 16).
- c. Numerical Models
 - i. Method of Characteristics Model, **MOC** (References 21, 22 and 23).
 - ii. Random Walk Solute Transport Model, **RWALK** (Reference 24).
 - iii. Modular 3-D Finite Difference Groundwater Model, **MODFLOW** (Reference 58).
 - iv. A Finite-Element Simulation Model for Saturated-Unsaturated Fluid-Density-Dependent Ground-Water Flow with Energy Transport or Chemical-Reactive Single-Species Solute Transport, **SUTRA** (Reference 60).
 - v. Computer Model of 2-D Contaminant Transport under the Influence of Oxygen Limited Biodegradation in Ground Water **BIOPLUME II** (Reference 59).

Several investigators have compared the performance of numerical codes to analytical solutions, benchmark data sets and real site applications (References 25, 26, 27, 28, and 29). The algorithm for choosing among the numerical codes is based, in part, on such comparisons. Another version of the algorithm is under development, capable of selection of transport models used to predict the effectiveness of alternative remediation schemes, optimizing for cost/effectiveness. In essence, the first algorithm suggests a model or models for the initial transport prediction; the second will provide guidance on the remediation method, and this may in turn require selection of another transport code.

The user responds to screen queries about whether analytical solutions are known to be appropriate or inappropriate (in the latter case, whether the region modeled is homogeneous or heterogeneous). If the complexities require a numerical model, the algorithm then jumps to that branch to select between the two available numerical codes. The flow charts identify the model recommended as a result of certain user responses: whether the subsurface waste disposal method is a landfill, a wastewater lagoon or spray irrigation; whether the flow is radial or not, whether the Dupuit approximation is valid or not; whether single or multiple sources are involved; whether full penetration analysis is adequate; whether regional flow is important or not. For example, the algorithm checks if a particular solution applies: if the user responds in the affirmative that flow in the region is strongly affected by pumping wells, then semianalytical (complex velocity potential) methods or complete numerical methods would be indicated as more appropriate than models based upon analytical solutions. In the case of selecting a numerical model, the user is prompted to respond to queries about grid size, longitudinal and transverse dispersion, whether the flow is parallel to the grid axes, whether storativity is significant, and whether any part of the aquifer changes from confined to unconfined flow or vice versa.

D. SCOPE OF THE USERS MANUAL

Although separate versions of the software are provided for the DOS and UNIX versions of the advisory system, and separate sections (III and IV) in this report describe a users guide to these versions, there are more similarities than differences between them. For example, both systems execute virtually the same models; the user interfaces and output formats vary to exploit the advantages of each operating system. Operating system considerations of more interest to programmers, such as the modular design of the software package and a file linkage guide, are discussed in Section V.

A workstation may include both surface and groundwater models, aimed at developing alternative remediation strategies for polluted surface and groundwater systems, and at designing the technical details of a preferred remedial action. The current versions of the modeling system support the following tasks:

1. Data management and analysis
2. Site characterization
3. Source identification
4. Plume delineation
5. Contaminant transport analysis
6. Risk analysis
7. Evaluation and optimization of potential remedial action alternatives, compliance monitoring, and sampling strategies.

When installed, its **hardware components** should include:

1. Graphics capability
2. Peripherals (e.g., printer, mouse)
3. Communication links (optional)
4. Storage devices

In designing the workstation, a flexible architecture was necessary for efficient updating, maintenance, and expansion of hardware and software. In addition, an operational support structure needs to be implemented for system maintenance and to provide user-application support. Finally, as an integral part of the organizational workstation environment, a continuing technology transfer program should be developed to include general introduction courses, various levels of on-site hands-on training, and roving experts visiting the different workstation locations on a regular basis.

SECTION II

INSTALLING THE ADVISORY SYSTEM

A. THE DOS ENVIRONMENT

The advisory system is supplied as a collection of a large number of executable files, DOS batch files, data files and utility files. These files (in compressed format), currently require four double-sided, high density (1.44 MB) 3.5-inch floppy diskettes, including an executable installation program (INSTALL) residing on Disk 1. The contents of these diskettes are intended to be loaded to a fixed hard-disk drive. When these files are uncompressed they occupy slightly over **12 MB** of storage space. Therefore, at least this amount of free space must be available on the user's workstation or personal computer. It is important to note that your computer must have already been loaded with the DOS device driver for extended graphics. If this is not the case, **DEVICE=C:\DOS\ANSI.SYS** should be added to the CONFIG.SYS file (usually, the operating system resides under the DOS subdirectory), and the computer re-booted in order to take advantage of all the graphics capabilities of both the computer and the software package, **before even invoking the installation program**. It is also highly recommended that a numerical coprocessor be installed on the hardware. Otherwise, the user will be waiting a long time for the results of the numerical prediction models and the stochastic simulations. Other technical programming considerations not essential for system installation purposes are discussed in Section V.

Loading is accomplished automatically by placing Disk 1 in any 3.5-inch drive, switching to that drive (from which the advisory system will be loaded to the hard disk drive), then typing INSTALL at the prompt. The user should then follow directions supplied by the installation program for information on the desired drives and subdirectories, etc. The installation program prompts the user for each of the other 3 diskettes at the appropriate time. Figure 1 displays the introductory screen of the installation program. Creating a separate directory on the hard drive for the advisory system is highly recommended. Therefore, a PATH must be specified so that the computer operating system can access your DOS library. Entry to the groundwater modeling system is obtained by invoking a batch file: GW.BAT. The user can readily create an access route to the advisory system from the main directory. For instance, if the system occupies a sub-directory named AFGWADV on drive C: the user can create a batch file to initiate the system as follows:

```
C:
CD\AFGWADV
PATH=C:\DOS;C:\;
GW
```

where for "C:\DOS" the user should substitute the name of the directory containing the DOS library, and "C:\\" is the root directory. The user may also want to edit the path statement contents in the AUTOEXEC.BAT file to include the AFGWADV subdirectory.

Exit from the system is accomplished by selecting Option "Z" in the Level 1 menu, which also cancels the current screen attributes.

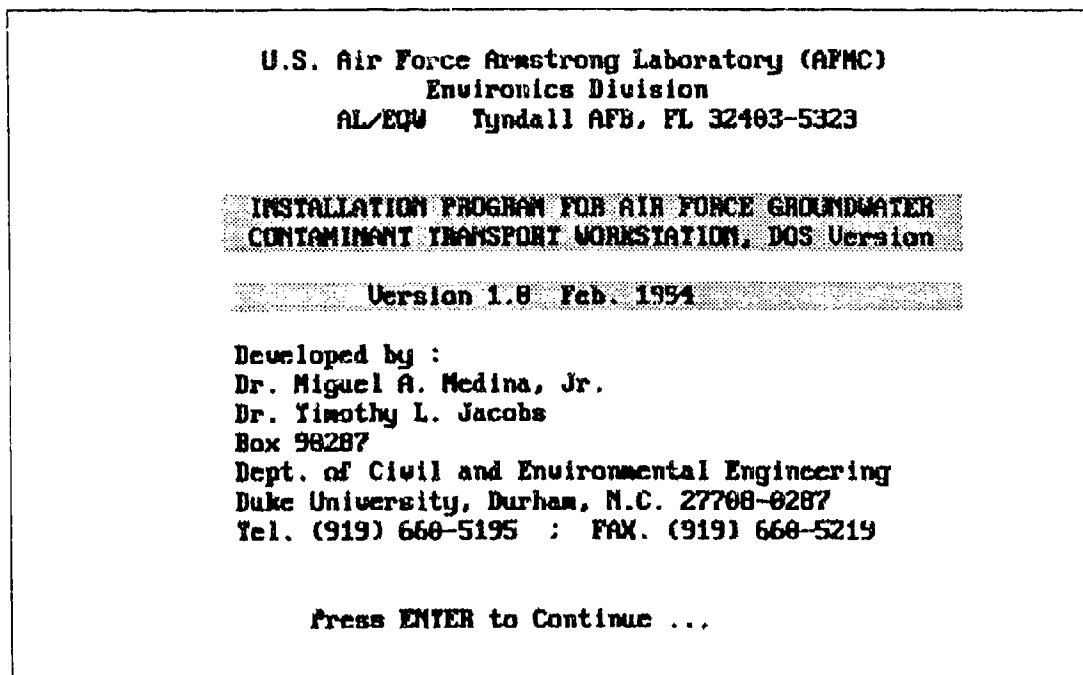


Figure 3. Introductory Installation Program Screen

B. THE UNIX ENVIRONMENT

Installation of the UNIX version of the advisory system involves six steps and can be accomplished via INTERNET transfer of the Advisory System source files. The UNIX version of the Advisory System requires the use of *Open Windows* version OS 2.1.1 or greater and a standard *FORTRAN 77* and *C* compiler. The UNIX version of the Advisory System requires 26.7 MB of disk space and includes all source code, graphics files, data input files and executable files. However, this memory requirement does not include space requirements for *Open Windows* and the *FORTRAN 77* and *C* compilers. Three *makefiles* are used to install the Advisory System. Each of these files provides compilation instructions for many subroutines included in the source code. These installation instructions assume the user is familiar with the basic commands and tools

of the UNIX operating system.

Each of the necessary installation steps is described in detail below. Throughout the installation instructions, the UNIX operating system prompt is defined as "%>".

1. To begin, 10 subdirectories need to be created within the directory where the system will reside, for example "gwadv". Create the subdirectories listed below using the "mkdir" command. First create the directory "gwadv" in the home directory using the command:

```
%>mkdir gwadv
```

Once the directory "gwadv" is created, move into that directory using the "cd" command:

```
%>cd gwadv
```

Now create the following subdirectories within the "gwadv" directory:

```
src
monca
graphics
modflow
sutra
graphics/src
graphics/demo
graphics/util
modflow/src
sutra/src
```

2. The second step in the installation process is to copy the source codes and makefiles for the Advisory System into the appropriate subdirectories created in step 1. Table 1 contains a list of all the source code files and makefiles used by the Advisory System. Each of the files can be copied from the tape drive or floppy disk using the "cp" command or over the INTERNET using the file transfer program ("ftp"). The user should consult the workstation guide for directions on copying from floppy disks or tapes to the hard drive.
3. Create the object file "syscall.o" file using the "make" command:

```
%>make -f makefile1
```

The makefile will automatically compile the appropriate files and place them in the proper subdirectory.

4. Create the graphics object files in the subdirectory "graphics" using the "make" command:

```
%>make -f makefile2
```

Again, the file compilation and organization are automatic.

5. Compile each of the FORTRAN subroutines using the following two commands:

```
%>chmod 755 makefile.bat
```

```
%>makefile.bat
```

6. The Advisory System is now installed and should be ready to execute. To start the Advisory System, type the command:

```
%>gwadv
```

Other technical programming considerations not essential for system installation purposes are discussed in Section V. Specific model use instructions are provided in Section IV.

Table 1. List of UNIX Version Source Codes and Makefiles

FORTRAN SOURCE CODES under /gwadv/src:					
epasf2.f	premoc.f	rndwlk.f	epasf3.f	premoc3.f	
ansi.f	epasf4.f	lgrd.f	preodast.f	scen.f	
att.f	ltird.f	preres.f	scrnc.f	attn.f	
pretdest.f	choice.f	odast.f	prewalk.f	preltird.f	
tdast.f	help1.f	psthlp.f	dupvg.f	help2.f	
plum2d.f	ran.f	epagw1.f	help3.f	plum2d2.f	
epagw2.f	help4.f	postplt.f	relib1d.f	epasf1.f	
rwalk2.f	help5.f	gwadv.f	param.f	ressq.f	
FORTRAN SOURCE CODES under /gwadv/Monca:					
MOCMC.f	cov.f	mainn.f	parlodmc.f	premain.f	move.f
					velo.f
					outpt.f
GRAPHIC SOURCE CODES under /grpahics/src:					
Dlvax.m4	grclos.m4	grfil3.m4	grlin1.m4	grply3.m4	outpt.m4
GPR.m4	grcol2.m4	grflip.m4	grline.m4	grprnt.m4	parlod.m4
Grde44.m4	grcol3.m4	grgrey.m4	grloct.m4	grscal.m4	postdest.m4
Grdem1.m4	grcolr.m4	grgri1.m4	grmesg.m4	grscpt.m4	postepa.m4
Grdem2.m4	grcon1.m4	grgrid.m4	grmode.m4	grsfac.m4	postplt.m4
Grdem3.m4	grcont.m4	grinit.m4	grmon2.m4	grsset.m4	project.m4
Grtest.m4	grctrl.m4	grinpa.m4	grmon3.m4	grsymb.m4	relib1d2.m4
MOC.m4	grcube.m4	grinpf.m4	grmov1.m4	grthr1.m4	odast.m4
SGL.m4	grcurs.m4	grinpi.m4	grmov2.m4	grline.m4	grklst.m4
grcutt.m4	grkey1.m4	grmov3.m4	grtime.m4	statis.m4	Xnewsys.c
gralst.m4	grdash.m4	grkey2.m4	grmovy.m4	grtran.m4	syscall.c
granot.m4	grdrw2.m4	grkey3.m4	grnear.m4	grvalu.m4	graphic.m4
grdrw3.m4	grkli1.m4	grper1.m4	grvec1.m4	graxes.m4	grdump.m4
grklin.m4	grpers.m4	grvect.m4	grfil.m4	greror.m4	groomn.inc
grplst.m4	grcler.m4	grfil2.m4	grkpla.m4	grply2.m4	
MAKEFILES:					
makefile	makefil1	makefil2	makefile.dat		

Table 1. List of UNIX Version Source Codes and Makefiles (Cont'd)

FORTRAN SOURCE CODES under /sutra/src :					
main.f	mgenrec.f	presutra.f	subs2.f		
mgenrad.f	pbcgen.f	subs1.f	usubs.f		
TEXT files under /graphics :					
grafic.doc					
FORTRAN SOURCE CODES under /graphics/util :					
Newsys.m4					
FORTRAN SOURCE CODES under /modflow/src :					
bas1.f	drn1.f	ghb1.f	modint.f	riv1.f	str1.f
bcf2.f	evt1.f	ibs1.f	pcg2.f	sip1.f	utl1.f
chd1.f	gfd1.f	main1.f	rch1.f	sor1.f	wel1.f
premod.m4	premod.inc				
TEXT FILES under /gwadv :					
moc7.d	rnwal1.d	rnwal9.d	sutr16.d	sutra8.d	odast1.d
moc8.d	rnwal2.d	rnwalk.d	sutra1.d	sutra9.d	odast2.d
moc1.d	rnwal3.d	sutr10.d	sutra2.d	tdast1.d	plum1.d
moc2.d	rnwal4.d	sutr11.d	sutra3.d	tdast2.d	rnoc6.d
moc3.d	rnwal5.d	sutr12.d	sutra4.d	sutr15.d	ressq3.d
moc4.d	ressq1.d	rnwal6.d	sutr13.d	sutra5.d	rnwal8.d
moc5.d	ressq2.d	rnwal7.d	sutr14.d	sutra6.d	sutr7.d
makefile.doc					

SECTION III

USERS GUIDE FOR THE DOS VERSION

This section provides a detailed guide to the use of the Advisory System, as presently implemented, in the DOS version. The intended audience is a user reasonably familiar with the general theory of contaminant transport in porous media and the DOS operating system, but who may not have experience with a given transport model. The general structure of this section is as follows: first, a "generic" guide is provided to the use of the system, which will be generally applicable regardless of the particular contaminant transport model chosen, presented in subsections A, B, and C. The subsequent sections present more detailed information on particular models, including a model selection algorithm, CHOICE.

For each model, notes are provided on: the applicability of a given model, the inherent limitations of a particular modeling approach, data preparation and output. Four applications of specific models are presented in subsection III(G).

A. STARTING THE SYSTEM

It is assumed that the system has been properly installed, according to the instructions provided in Section II(A), on a fixed disk drive in a properly configured personal computer or workstation. Switching to the appropriate subdirectory containing the software package, the system is then started by simply typing 'GW'. This will result in an introductory screen identifying the current version the system (Figure 4), followed by a symbolic demonstration of contaminant transport and remediation.

B. FILE MANAGEMENT

The first task is identifying the site being studied, and setting up the needed disk files. Beyond the introductory screen and demonstration, the user is presented with the menu shown in Figure 5. Option 1 provides a simple introduction. If the site indicated is a previously analyzed site (Option 2), the system will locate all existing files. On the other hand, if the site is a new site, the system will check to make sure that files with the user-supplied names do not already exist. Appropriate options will be presented if these conditions are found to be violated. For a previously analyzed site, the user is prompted to select a file name from the existing data files. The user needs to fill in a 7-character file name which includes the site name and model ID. The latter should consist of 2 digits, and the site name should consist of 5 letters. The site name and model ID are used to identify files associated with the site and the model applied previously to that site. The user then goes to Level 1 and Option E (Analyze a previously analyzed site). Figure 6 provides an example for a previously analyzed site.

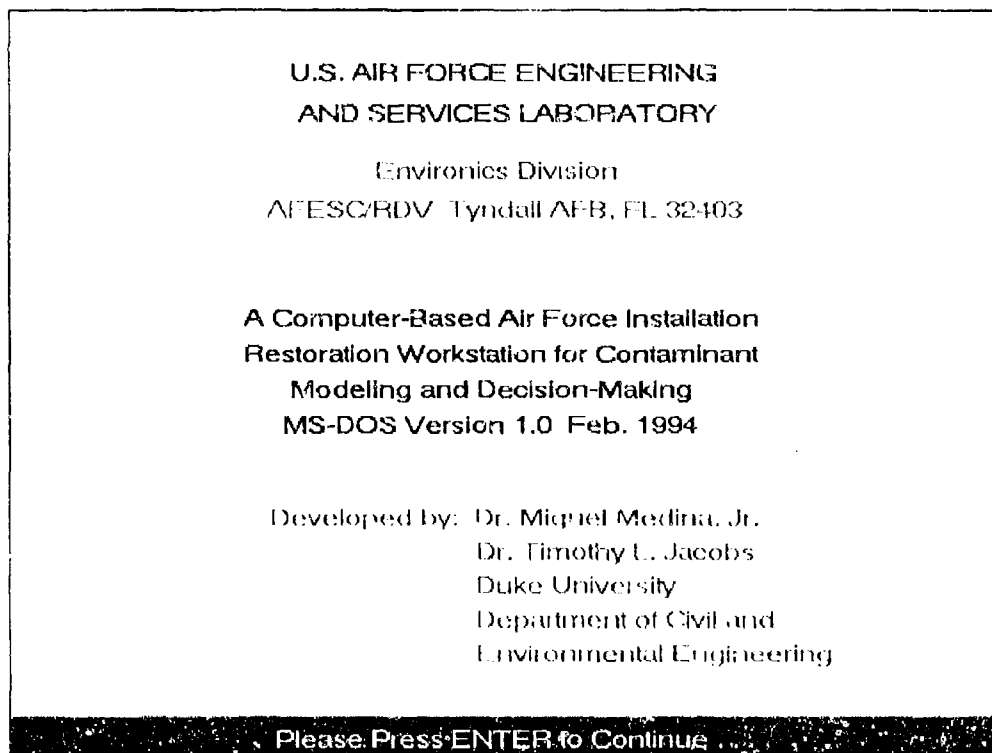


Figure 4. Introductory Screen

The new site analysis option obviously provides the user with the option to begin a new analysis. It can also be chosen to reanalyze a site with completely new data. The user needs to enter a five-character site name. After entering the site name, this option is completed by entering a header, identifying the analyst, date, and title of the project. The system then proceeds to Level 1.

Option 5 is provided so that those without experience in the operation of the system can avoid having to create data files on the system. The system uses default site name 'PRIOR' to create the necessary input and output files.

C. Level 1, Master Menu

After setting up the files, the system proceeds to Level 1, which controls the pathways to the whole system. Upon accessing Level 1, a selection menu will be displayed (Figure 7).

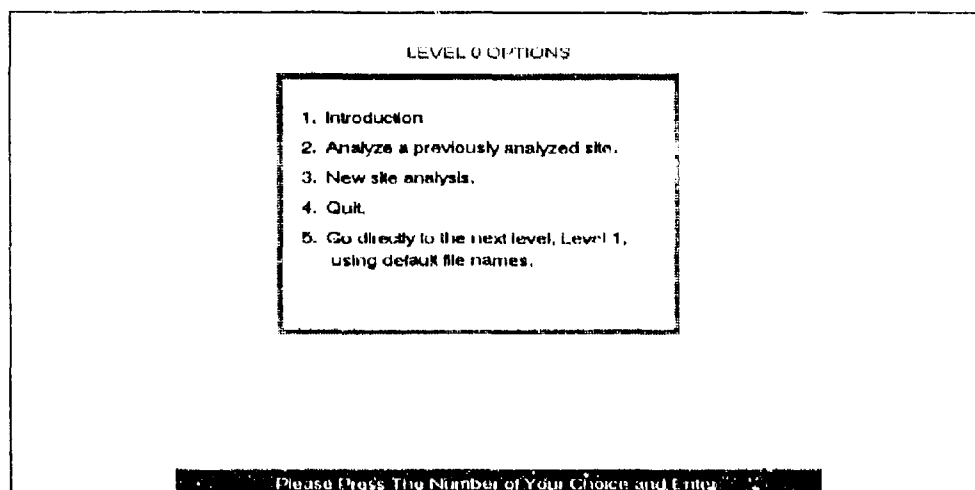


Figure 5. Level 0 Options

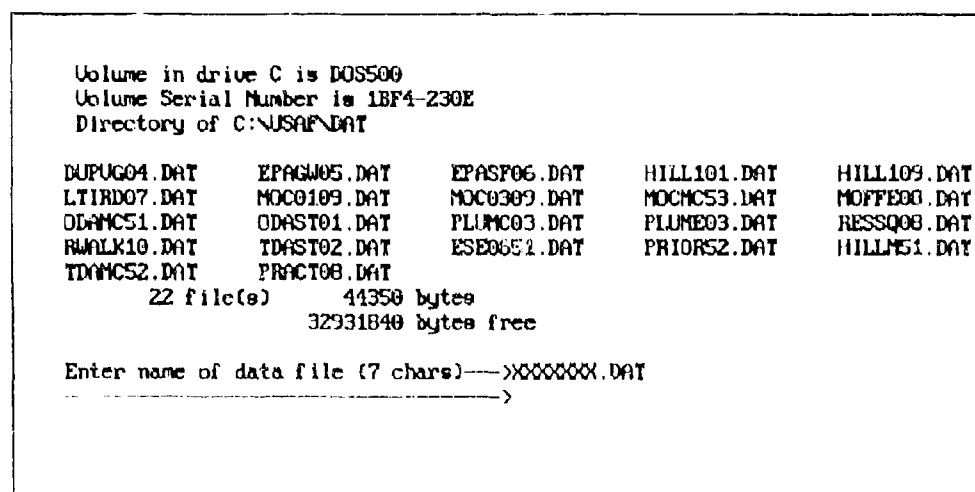


Figure 6. An Example of File Management

The options presented here are divided into two categories: "Advisory support" and "File Utilities." The utilities are self explanatory, and helpful for file management. The option of advisory support opens the gates to either a preliminary analysis or access to all the other models. Figure 8 illustrates file utilities.

```

LEVEL 1 OPTIONS

ADVISORY SUPPORT
A: LeGrand Method for Preliminary Analysis
B: Impact Scenario Definition
C: Algorithm for Model Selection, CHOICE
D: Direct Selection of Model
E: Analyze a Previously Analyzed Site
O: Uncertainty Analysis and Optimization

FILE UTILITY
L: Display Directory of Data and Output Files
P: Print Current Output File
S: Scroll Output File to Screen
T: Use MS-DOS Editor to View Output File
R: Start New Analysis: Goto Level 0
Z: Abandon Analysis: Exit to DOS

Please Press the Character of Your Choice, and Enter:

```

Figure 7. Menu for Level 1

D. Preliminary Analysis

In many cases it may appear to the analyst that a proposed site is so poorly situated that it cannot be analyzed with detailed modeling. In other cases, some sites may need preliminary analysis to evaluate the hydrogeology and provide a guide to further data collection. To formalize this subjective process we have provided for preliminary analysis using the LeGrand method. In most cases, the first stage of analysis should thus be to apply this model (Option A): further details of utilizing the LeGrand method are presented below.

In the early stage of site investigation, project managers usually lack the manpower to conduct detailed modeling analyses of all sites that may have a potential effect on groundwater. In some instances a proposed site will have such a poor hydrogeologic setting that a preliminary analysis is necessary to guide the further investigation. Conversely, some cases will have such a low degree of contaminant severity and potential risk of contamination that a site could be passed without detailed modeling. Often such decisions are made subjectively. However, it is safer and more desirable to establish formal criteria for the bypassing of detailed modeling on a given site.

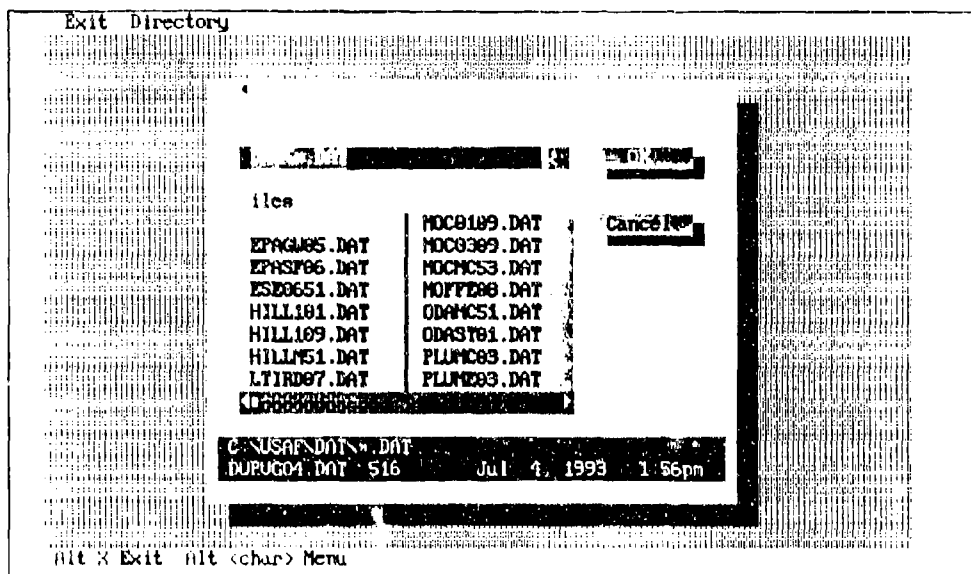


Figure 8. Display Directory of Data and Output Files

In the advisory system, criteria for this preliminary screening may be formalized by use of the screening analysis developed by LeGrand (1983), which requires only readily available site-specific data. This approach is essentially a numerical rating system for evaluating the potential of ground water contamination from waste disposal sites. The system focuses on weighting four key geologic and hydrologic characteristics in the vicinity of contamination sources. The key parameters used are: 1) distance to a water supply or perimeter of compliance; 2) depth to water table; 3) hydraulic gradient; and 4) permeability-sorption, as indicated by the geologic setting. In a second stage, attention is paid to the type and severity of the generalized contaminants associated with the use of the site. Weighting and integrating the site and contaminant characteristics then yields a numerical situation rating.

The LeGrand method may be used to evaluate hydrogeology alone, or extended to include consideration of the type of waste disposal site (PAR rating). When both analyses are undertaken these are combined to provide a combined situation rating. This combined situation rating can be used for the preliminary decision. Output of the model includes a shorthand summary of the analysis, as in the following example:

```

Description 21- 3936ABWD +E
PAR          18    5
-----
+ 3    +1    =    + 4 E

```

The first line given above (Description) summarizes the analysis of site hydrogeology. Higher numbers here (on a scale of 0-9) indicate less favorable characteristics, so these may readily be identified from the description. In the analysis given above, the entries in the Description line indicate the following:

- 21 Total rating (sum of next four digits)
-
- 3 Distance from source to point of impact.
- 9 Depth to water table.
- 3 Water table gradient.
- 6 Permeability-sorption.
- A Letter identifier of permeability-sorption.
- B Degree of confidence in estimates.
- W Indicates measured in relation to a well.
- D Special identifier.
- + E Hydrogeologic grade.

In this case, the hydrogeologic rating is in the poor range (E) because the total rating is > 20 . Analysis of the digits shows that the most important factor contributing to this poor rating is the depth to water table below the contamination source. The second line (PAR rating) is obtained from a hazard potential matrix. In this case higher values indicate decreasing contaminant severity and/or decreasing aquifer sensitivity. The combined situation rating is then obtained by subtracting the PAR rating from the hydrogeologic rating.

LeGrand's method has been directly interpreted into an interactive program for inclusion into the system. Preliminary judgment is then based on the following criteria (which may be altered): for a combined situation rating of $< - 8$ a site is judged probably acceptable, without further analysis, while for a situation rating $> +4$ a site is judged probably unacceptable. In the uncertain range from $- 8$ to $+ 4$ further modeling is recommended with actual transport models.

The great advantage of the LeGrand method is thus in providing a standardized weighting system that is broadly applicable, yet quick and easy to apply. Such analysis does not form the basis of a final recommendation, except in the extreme cases of very low contamination probability or very high contamination probability. The LeGrand method provides an effective means of identifying such cases. However, in all cases the user is free to proceed to more detailed analysis through actual modeling of contaminant transport. For instance, even where a very low probability of contamination is indicated by the LeGrand analysis, the user may wish to proceed to more detailed modeling if the contaminant in question is particularly hazardous.

The LeGrand method is carefully designed to have a wide degree of applicability, and will be an effective tool for preliminary analysis in most situations. Its effectiveness

is limited primarily by the fact that it is designed as a preliminary analysis tool, and, probably in the majority of cases, the model will not provide a definitive answer. The user should of course realize that the method treats site hydrogeology in only a generalized manner. Where more specific details of the hydrogeology are known, the user should take these into account in analyzing the model results.

Data input for the LeGrand method is interactive. The user may choose to rate site hydrogeology only (Stage 1) or continue analysis with consideration of the PAR rating (Stage 2). On completion the user has the option of re-analyzing the site. It will often be desirable to rate a site in regard to several different potential points of impact, and with consideration of varying degrees of engineering modifications.

In Stage 1 the following data are requested:

Step 1.

Choose distance on ground between site and nearest water supply (or specified boundary) from the following choices.

	(feet)	(meters)
0	> 6200 ft.	> 2000 m
1	3100 - 6200	1000 - 2000
2	1001 - 3100	300 - 999
3	501 - 1000	150 - 299
4	251 - 500	75 - 149
5	161 - 250	50 - 74
6	101 - 160	35 - 49
7	61 - 100	20 - 34
8	31 - 60	10 - 19
9	0 - 30	0 - 9

When the water table lies in permeable consolidated rocks, 6 points are allotted on the distance scale; in poorly permeable rocks, 4 points are allowed.

Step 2.

Estimate the shallowest depth to the water table below the base of the contamination source more than 5% of the year from the choices below.

	(feet)	(meters)
0	> 200 feet	> 60 meters
1	91 - 200	30 - 60
2	61 - 90	20 - 29
3	36 - 60	12 - 19
4	26 - 35	8 - 11
5	16 - 25	5 - 7
6	9 - 15	3 - 4
7	3 - 8	2.5 - 1.5
8	1 - 2	1 - 0.5
9	< 1	< 0.5

When the water table lies in permeable or moderately permeable consolidated rocks 6 points are allotted - in poorly permeable rocks 4 points are allotted.

Step 3.

Choose the most appropriate description of the general water table gradient from the following table:

- | | |
|---|------------------------------------------------------------------------------------------------------------|
| 0 | Gradient away from all water supplies that are located closer than 1000 meters from the site. |
| 1 | Gradient is almost flat. |
| 2 | A gradient of less than 2% exists towards the water supply, but this is not anticipated direction of flow. |
| 3 | Gradient less than 2% towards the water supply, and this is the anticipated direction of flow. |
| 4 | Gradient greater than 2% towards the water supply, but this is not the anticipated direction of flow. |
| 5 | Gradient greater than 2% towards the water supply, and this is the anticipated direction of flow. |

Step 4.

In step 4 a digit and letter identifier describing permeability-sorption for the site is chosen from Table 2.

Step 5.

Indicate degree of confidence in accuracy of values:

- A: Confidence in estimates of values for the parameters is high and estimated values are considered to be fairly accurate.
- B: Confidence in estimates of values for the parameters is fair.
- C: Confidence in estimates of values for the parameters is low and estimated values are not to be considered accurate.

Table 2. Selection of Permeability-Sorption Indicators for the LeGrand Model
(for unconsolidated material)

material	clay	clay with more than 50% sand	sand with 15- 30% clay	sand with less than 15% clay	clean fine sand	clean gravel or coarse sand
category	I II	I II	I II	I II	I II	I II
thickness > 95 (in ft)	0A 0A	2A 2A	4A 4A	6A 6A	8A 8A	9A 9A
75-94	0B 1C	1D 2F	3E 4G	5F 6E	7E 8E	9G 9M
60-74	0C 2C	1E 3D	4D 5E	5G 6F	7G 8F	9H 9N
46-59	0D 3B	1F 4C	4E 6C	5H 7D	7H 8G	9I 9O
28-45	0E 4B	2D 5B	4F 6D	5I 7E	7I 9D	9J 9P
10-27	1B 6B	2E 7B	5C 7C	5J 8D	7J 9E	9K 9Q
< 10	2B 8B	3C 8C	5D 9B	5K 9C	7K 9F	9L 9R

For bedrock at land surface, use 5Z for category I, 9Z for category II.

Category I - unconsolidated material overlies shale or other poorly permeable rock.

Category II - unconsolidated material overlies permeable consolidated rock (fractured or jointed igneous or metamorphic rocks, cavernous carbonate rocks and faults).

Step 6A.

Distance from contamination source is measured to:

W: a well.

S: a stream or perennial spring.

B: a property boundary or perimeter of compliance.

Step 6B.

Up to two additional letter identifiers may be selected from the following list:

C : SPECIAL CONDITIONS REQUIRE THAT A COMMENT OR EXPLANATION BE ADDED TO THE EVALUATION.

D: CONE OF PUMPING DEPRESSION NEAR A SOURCE OF CONTAMINATION. THIS MAY CAUSE DIVERSION TOWARD PUMPED WELL.

E: DISTANCE RECORDED IS THAT FROM A WATER SUPPLY (OR BOUNDARY) TO THE EDGE OF AN EXISTING PLUME RATHER THAN ORIGINAL CONTAMINANT SOURCE.

- F: SOURCE IS LOCATED ON A GROUNDWATER DISCHARGE AREA, SUCH AS A FLOOD PLAIN, WHERE MINIMAL GROUNDWATER INTRUSION IS EXPECTED.
- K: SITE LOCATED IN KARST TYPOGRAPHY, OR IS UNDERLAIN BY CAVERNOUS LIMESTONE.
- M: MOUNDING OF THE WATER TABLE BENEATH A CONTAMINATION SITE - COMMON BENEATH WASTE SITES WITH LIQUID INPUT.
- P: PERCOLATION MAY NOT BE ADEQUATE FOR SITE. THE PERMEABILITY -SORPTION DIGIT SUGGESTS THE DEGREE TO WHICH PERCOLATION MAY BE A PROBLEM, A DIGIT OF 3 OR LESS BEING A SPECIAL WARNING OF POOR PERCOLATION.
- Q: DESIGNATES A "RECHARGE OR TRANSMISSION" PART OF AN EXTENSIVE AQUIFER THAT IS SENSITIVE TO CONTAMINATION. MAY BE SUGGESTED BY A HIGH VALUE ON THE PERMEABILITY-SORPTION SCALE.
- R: RADIAL OR PARTIAL RADIAL FLOW FROM A HIGH WATER-TABLE POSITION. (TWO OR MORE SITE RATINGS MAY BE NEEDED).
- T: INDICATES THAT THE WATER TABLE IS IN FRACTURED OR CAVERNOUS ROCK.
- Y: ONE OR MORE CONFINED (ARTESIAN) AQUIFERS UNDERLIE THE WATER TABLE AQUIFER.

In Stage 2 of the LeGrand analysis the user must enter information relating to the contaminant severity and aquifer sensitivity. This information is best read from the PAR matrix diagram provided in LeGrand (1983). However, the option is also provided to estimate these values in response to a series of queries.

E. ACCESS TO MODELS

Access to contaminant transport models is provided by requesting assistance in model selection (the Choice algorithm) or by direct model selection by the user.

1. Model Selection Algorithm

The objective of the Choice Algorithm is to consider a wide range of groundwater modeling situations, and, in each case to determine whether there is an appropriate analytical solution available with which Monte Carlo analysis of the risk associated with the site can be analyzed. Where such a solution is not available, in some instances semi-analytical methods will be appropriate for preliminary analysis. Otherwise, one may need to proceed to more complex numerical models for analysis of the site.

The introductory screen of the Choice Algorithm is illustrated in Figure 9. The logic employed in this algorithm is given in detailed flow chart form in the first technical report (Medina and Jacobs, 1993). The first menu of the algorithm is presented in Figure 10. If the user selects choice 5 from the menu, the next screen (Figure 11) prompts the user for responses in order to determine if analytical solutions are inadequate.

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HYDROGEOLOGICAL MODEL SELECTION
 CONTAMINATION RISK ANALYSIS
 CHOICE ALGORITHM

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 Duke University
 Department of Civil and
 Environmental Engineering

Press ENTER to Continue ...

Figure 9. Choice Algorithm

This module aids in selection of a model appropriate for the site hydrogeology and method of disposal of the wastes. It is applicable for either deterministic or Monte Carlo analysis of the contamination risk. The selection process evaluates models based upon analytical, semi-analytical and fully numerical solutions to the governing equations, subject to appropriate initial and boundary conditions. The selection of models may be accomplished with available data or qualitative information on the waste site.

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ENTER your selection:

Figure 10. First Menu of CHOICE Algorithm

CHECK if ANALYTICAL SOLUTION is clearly inappropriate according to currently available data.

1. The horizontal extent of the region of interest in the aquifer is KNOWN to be near (say 250 ft.) to a distinct hydrogeologic boundary, such as an intersecting river, aquitard or distinct inhomogeneity in the medium.
2. The region of interest is in an aquifer that is distinct from the aquifer directly affected by the site. For example, a site may impact a shallow water table aquifer while the region of interest for modeling is in an underlying system separated by an aquitard.
3. Contaminant of interest is an immiscible liquid in water or has a specific gravity significantly different from that of water.
4. Flow in the vicinity of the site is strongly affected by pumping wells or other hydraulic controls.
5. Impacted aquifer is a fractured rock system.
6. Source input must be treated as a slug injection.
7. NONE OF THE ABOVE apply.

ENTER your selection:

Figure 11. Query On Applicability of Analytical Solutions

If the user responds with choice 4 (flow strongly affected by pumping wells), then models based upon analytical solutions are clearly inappropriate, and the next screen checks for the utility of semianalytical solutions.

Check for utility of semi-analytical solutions:

1. Aquifer can be characterized as not drastically inhomogeneous in region of interest, but may be affected by constant head boundaries or pumping wells. Sources may be points, ponds or wells.
2. Systems other than as described in 1.

ENTER your selection:

Figure 12. Applicability of Semi-Analytical Solutions

For complex inhomogeneous systems, the user would select (2.), and the algorithm would then proceed to the numerical models (Figure 13).

Complex conditions at the site require analysis with a numerical model. The options include MOC and RANDOM WALK. RANDOM WALK has a 40x40 maximum grid size. The MOC grid has a 20x20 limit for solute transport. Select the most representative site condition below.

1. A variable grid size is required up to 100x100.
2. Due to the aquifer size, the grid extends in the Y or Z direction must be larger than 10 times the transverse dimensions of the plume.
3. The ratio of longitudinal to transverse dispersivity is greater than 10.
4. Flow patterns are likely to be predominant in one or two parallel to the grid axes.
5. The storage coefficient varies significantly over the area to be modeled.
6. Hydrogeology changes from confined to water table or vice versa during the simulation in all or part of the aquifer.
7. None of the above apply.

Enter selection -->

Figure 13. Selection Among Two Numerical Models

In many permitting applications use of a contaminant transport model to analyze contamination risk will require estimation of the rate of leaching from a source, which is itself a complex phenomenon. To provide for calculation of leaching rates, the Hydrologic Evaluation of Landfill Performance (HELP) Model (Schroeder et al., 1984) is provided. This program was developed to facilitate rapid, economical estimation of the amounts of surface runoff, subsurface drainage and leachate that may be expected to result from the operation of a wide variety of possible landfill designs. Thus the authors caution that the model "should not be expected to produce credible results from input unrepresentative of landfills." The Choice Algorithm thus includes the option of calling the HELP model to establish leaching rates, modified to allow a fixed amount of rainfall so that the model can provide a rough simulation of leaching resulting from spray irrigation. In these calculations the results can also be used to calculate a rough, conservative approximation of vadose zone attenuation, given knowledge on the half-life and distribution coefficient of the contaminant species.

An important limitation of the HELP model is its assumption that the layers in the design are horizontally uniform. This assumption may not be valid for some larger sites. Further, the method has not been tested for types of sites other than hazardous waste landfills. When used in such situations the model output should be carefully examined and compared to estimates derived from other sources.

Other limitations are inherent in the simplifying assumptions used in the model development. These are primarily of importance in relation to calculation of daily and peak values (which are generally not of direct concern in the application of analytical ground water transport models). Infiltration through the surface is computed using the SCS runoff curve number technique. The actual rainfall intensity, duration and distribution are not considered. Factors such as slope and surface roughness, which would be important if individual rainfall or storm events were used, are considered only in the context of the land management factors used in the selection of the SCS runoff curve number. In calculation of evapotranspiration, the model does not use actual daily temperature and solar radiation values. Instead, mean daily temperature and solar radiation data are used. Similarly, daily leaf area indices are interpolated from 13 values scattered throughout the year. As a result, calculated daily evapotranspiration values may be quite different from actual daily values. However, computed and actual monthly and annual totals of the daily evapotranspiration should be similar.

The model also assumes that the characteristics of the landfill do not change with age, and that the only effect of vegetation on the soil characteristics are those shown through the SCS runoff curve number. Barrier soil layers are assumed to remain saturated, and percolation through barrier layers is not restricted or aided by segments below the barrier soil. Finally, the model assumes that surface runoff does not occur, and that the water table is below the landfill. In summary, the HELP model represents a compromise to reduce the difficult question of hydrologic performance of a landfill to a manageable scale. Data input for the HELP model is interactive. When the program starts it first prints a header, and then asks the following:

DO YOU WANT TO ENTER OR CHECK DATA OR TO OBTAIN OUTPUT?

ENTER 1 FOR CLIMATOLOGIC INPUT,

2 FOR SOIL OR DESIGN DATA INPUT,

3 TO RUN THE SIMULATION AND OBTAIN DETAILED OUTPUT,

4 TO STOP THE PROGRAM, AND

5 TO RUN THE SIMULATION AND OBTAIN ONLY SUMMARY OUTPUT.

The program will return to this question each time it completes a portion of the program. For use in the advisory system the user will typically wish to enter soil or design input data (2), enter climatologic data (1), and then run the simulation to obtain only summary output (5). Choosing (4) will result in exiting from HELP, then proceeding to any of the other transport models requested.

2. Direct Selection of Models

The system also provides an option for direct user selection of a model. For the more sophisticated users, this is the most efficient way to gain access to a specific model. The direct selection menu is presented in Figure 14.

MENU OF MODELS

ANALYTICAL MODELS

1. Odast: 1-D transport model
2. Tdast: 2-D transport model
3. Plum2d: 2-D transport model
4. DUPVG: 2-D transport model, unconfined
5. EPAGW: 3-D EPA Monte Carlo transport model
6. EPASF: EPA Monte Carlo...Impact on surface water
7. LTIRD: 2-D radial transport model

SEMI-ANALYTICAL MODELS

8. RESSQ: 2-D complex velocity potential model

NUMERICAL MODELS

9. USGS MOC: Method of Characteristics model
10. RNDWLK: Random Walk solute transport model
11. USGS MODFLOW: 3-D flow model
12. USGS SUTRA: 2-D transport model
13. BIOPLUME II: 2-D transport model
14. EXIT TO MAIN MENU

Please Press The Number of Your Choice and Enter

Figure 14. Menu for Direct Selection of Models

Figure 15 presents the menu for uncertainty analysis and optimization. Once a specific transport model is selected, an estimate of the distribution of the contaminant concentration is needed to assess the risk associated with a site. A major problem in determining the risks of any site is related to the uncertainties associated with model parameters such as the leachate release concentration, and the hydraulic conductivity. In most cases only the mean and variance of the distributions of the individual parameters are known. To incorporate model parameter uncertainties, approximate solution techniques may be used. Mathematical simulation and Monte-Carlo simulation are used to estimate the output distributions. A probabilistic assessment of the groundwater contaminant concentration and its corresponding error can then be used to address the risks associated with a specific site. Regulatory actions or remedial decisions based on this approach can be significantly different and more realistic from those based on a deterministic estimate of groundwater contaminant concentrations.

In the menu above, there are entries for five numerical models (three in addition to two previously documented by the authors in the first report, Reference): MODFLOW (McDonald and Harbaugh, 1988), SUTRA (Voss, 1984), and BIOPLUME II (Rifai, et al., 1987). These numerical models are included in the advisory system for the modeling of complex hydrogeological environments. These software packages are in the public domain and at least the first two are widely used in groundwater studies.

MODFLOW is a modular three-dimensional finite-difference groundwater flow model. It can be used to simulate two-dimensional areal or cross-sectional, and quasi- or fully-three-dimensional, transient flow in anisotropic, heterogeneous, layered aquifer systems. The program is written in modular form. It consists of a main routine and a series of highly independent subroutines called "modules." These modules are grouped into packages which address the general use of the model, specific features of the hydrologic system, or particular solution techniques.

SUTRA simulates fluid movement and the transport of either energy or dissolved substances in a saturated-unsaturated subsurface environment. The hybrid finite-element and integrated-finite-difference method is used to approximate the two-dimensional governing equations. SUTRA flow simulation may be employed for areal and cross-sectional modeling of saturated groundwater flow systems, and for cross-sectional modeling of unsaturated zone flow. Solute transport simulation may be employed to model natural or man-induced chemical species transport including processes of solute sorption, production and decay, and may be applied to groundwater contaminant transport problems and aquifer restoration designs.

BIOPLUME II is a two-dimensional model for simulation of transport of dissolved hydrocarbons under the influence of oxygen-limited biodegradation. The code also simulates reaeration and anaerobic biodegradation as a first order decay in hydrocarbon concentrations. The model is based on the 1987 version of the USGS two-dimensional method of characteristics transport model by Konikow and Bredehoeft. It computes the changes in concentration over time due to convection, dispersion, mixing, and biodegradation.

Once a model has been selected by either of the above processes, the system will proceed to run the model, automatically invoking the appropriate input data pre-processor. This is a program designed to facilitate preparation of the necessary data.

On exiting the preprocessor, control will shift to the actual transport model. If in Monte Carlo mode, you may be asked to input a random number seed at this stage. The model iterations will then be commenced, with an iteration counter displayed on the screen and a bell sounded when finished. Execution time is highly dependent on the particular model and data configuration. However, it is recommended that at least 500 Monte Carlo runs should be used to build up an accurate picture of the cumulative frequency of contamination risk.

MENU OF MODELS

UNCERTAINTY ANALYSIS MODELS

1. Odast in Monte Carlo mode: 1-D transport model
2. Tdast in Monte Carlo mode: 2-D transport model
3. USGS MOC in Monte Carlo mode

OPTIMIZATION MODELS

4. OPTIM: Optimization demo program
5. Optimization program for well location
6. EXIT TO MAIN MENU

Please Press The Number of Your Choice and Enter.

Figure 15. Uncertainty analysis and optimization

Following the successful completion of a model application several things will happen: the data will be stored or displayed as appropriate, graphics will be displayed, and finally the user will be returned to the Level 1 menu, with an option to rerun the last applied model. Note that this option will query whether the user wishes to change the contaminant studied and concentration level.

The graphics display will depend on whether the model has been run in the deterministic or Monte Carlo mode. In either case, plots are provided only for the last time step modeled, although data from each time step specified will be incorporated in the output file. In Monte Carlo mode, for each observation point the data will be sorted into ascending order and the probability of exceedance of the standard calculated. A cumulative frequency plot is then displayed.

In deterministic mode, a three-dimensional perspective plot of the contaminant plume will be displayed for the two-dimensional analytical solution models. However, this option is valid only if the grid dimensions are at least 2 x 2. This plot is interactive, and the user may display a regulatory standard level, and change color and fill design. Specifying a fill color of 0 results in a line drawing of the plot, which is usually best for obtaining a print on a single color printer. The user also has the option of recalculating the perspective plot after rotation, scaling or translation operations. The semi-analytical model, RESSQ, produces a special plot of the flow lines and pollutant fronts, followed by plots of concentration development at specified observation points.

F. INPUT/OUTPUT DATA FORMATS FOR SPECIFIC MODELS

In the following sections suggestions are provided on the use of component models in the system. In each case, the following items are addressed: 1) applications of the particular model, 2) limitations of the model's approach, and 3) details of data input and output.

1. ODAST

The program ODAST evaluates the one dimensional analytical solute transport solution considering convection, dispersion, decay and adsorption in porous media (Javandel et al., 1984). The program has been modified to facilitate Monte Carlo analysis. The solution method can thus handle many types of transport conditions, and is also numerically stable and executes very fast. The idealized situation from which the solution arises is as follows: the model considers an infinitely long column of a homogeneous isotropic porous medium, with a steady state uniform flow (constant seepage velocity). A particular solute is injected from one end of the system for a period of time such that the input concentration may vary as an exponential function of time. The value of concentration may then be calculated at any time t and distance x from the injection boundary. In the field, such an idealized situation could be represented by an infinitely long ditch of contaminated waste water fully penetrating an infinitely long confined aquifer, with the ditch cutting the aquifer perpendicular to the direction of flow.

The idealized situation described obviously does not exist in the real world. However, the solution provides a valid approximation in many cases. As with most analytical solutions the assumption is made of isotropic, uniform, steady state regional flow. This will often be a reasonable approximation of actual flow conditions. Likewise, the assumption of a confined aquifer may provide a reasonable approximation for analysis of phreatic aquifers if the flow regime is not strongly altered by the rate of fluid input from the source, and the saturated thickness remains approximately constant. Even where the saturated thickness is to some extent variable over time use of the average saturated thickness will enable analysis of average contamination risk. This approximation will be particularly valid for analysis in the Monte Carlo mode. In the Monte Carlo mode the input concentration and regional flow velocity both become random variables, and the cumulative frequency estimated over these and other random parameters should provide a reasonable estimate of the average risk. However, if the source itself contributes fluid that becomes an important factor of the flow regime (so that radial flow from the source is established), the confined aquifer assumption becomes inappropriate, and the phreatic surface will move in response to the source input. This condition is tested for in the CHOICE algorithm. Another model, DUPVG, may be appropriate under these conditions.

Real sources will not be of infinite length; however, the one dimensional solution provides a reasonable approximation for finite sources if the observation point is

sufficiently near the finite width source so that the effect of the source edges will be minimal. For instance, if a source has a lateral extent of 200 feet and the perimeter of compliance is 50 feet from the source, the one-dimensional solution is likely to provide a reasonable (and conservative) approximation of contamination risk along the axis extending from the center of the source (but not near the source edges). The exact distance to which the one dimensional solution can be carried downstream from a finite source without introduction of unacceptable error will depend on the interaction of all the forces controlling the flow regime.

The method can also be extended to cover input configurations other than the ideal ditch perpendicular to flow. Many situations of interest will involve large areal surface applications of wastes. Modeling the actual distribution of contamination in such cases is a complex process. However, solutions such as ODAST may be appropriate given certain assumptions. The first step is to calculate the rate of mass loading at the water table surface, after any vadose zone attenuation. We must then make the assumption that the substance is more or less instantly vertically mixed in the aquifer. Such an approximation is of course more valid for relatively thin surficial aquifers. (Generally, when the degree of vertical penetration is a significant factor in determining plume development, a three-dimensional solution, such as EPAGW, must be employed.) This constant areal input must then be represented as a line source at the downflow edge of the area. To do this one can make the simplifying assumption that the whole aquifer volume beneath the landfill is thoroughly mixed by the time flow reaches the downstream edge of the source, and calculate an edge concentration based on the loading diluted by the regional flow. (The concentration at the edge of the aquifer will thus have a maximum possible value equal to the leaching concentration.) Such an approach is most applicable where the loading is approximately constant over the whole area. (An alternative is to model the areal source as a Gaussian source, maximum at the center and declining towards the edges. This option is provided by EPAGW.) Model input provides options for calculating concentration in this manner, or for direct input of the concentration at the source edge.

The nature of the solution, and the additional assumptions that may be needed to employ it, as indicated above, introduce a number of **limitations** in the applicability of the model. First, ODAST is clearly inapplicable when the source cannot be modeled as laterally approximately infinite in terms of the point of interest. As with all analytical solutions, the model will not be appropriate where there is a significant deviation from the conditions of uniform, steady-state regional flow. However, minor violations of these conditions will not have important effects on the general analysis of contamination risk, and the model will also be valuable for initial analysis when non-uniform flow is suspected, but not fully documented. The solution also assumes a semi-infinite flow regime, and thus cannot take into account aquifer interactions with constant head boundaries, such as rivers. The CHOICE algorithm suggests avoiding use of this type of analytical solution when the perimeter of compliance or other point to be modeled is within 250 feet of a fixed head boundary. Limitations that are more difficult to assess

involve the assumptions that vertical concentration gradients can be ignored (full mixing), and that the source can be modeled as a uniform strength line. Clearly, the solution cannot be used for liquid contaminants that are not fully miscible and tend to float or sink within an aquifer. Further, ODAST may result in underestimation of contaminant risk at the aquifer surface if full mixing does not occur.

The preprocessor developed for ODAST is in a user-friendly format that is used for most of the models in the system. This consists of presentation of a number of screens, with input slots to be filled. The data to be input for ODAST are as follows:

NUMX: Number of points modeled in the X direction, which establishes the 1-dimensional grid. From 1-18 points may be used. Grid size does not affect solution. The X direction is coincident with the regional flow vector.

NUMT: Number of time steps for calculation.

DL: Longitudinal dispersion coefficient.

V0: Mean pore water velocity of the regional flow. This can be estimated from the average observed flow velocity, v , as $V_0 = v/P$, where P is the porosity of the medium.

R: retardation coefficient, $= v/v_c$, where v is the velocity of the regional flow and v_c the apparent velocity of the contaminant. If we assume reversible linear adsorption, R can be estimated as:

$$R = 1 + \frac{K_d \rho_b}{\phi} \quad (1)$$

where K_d is the soil-water distribution coefficient, ρ_b is the soil bulk density and ϕ is porosity. For this model, soil bulk densities are not explicitly considered, and the user must input a computed value for R . The value of K_d will also vary with the type of the medium, particularly the organic carbon fraction of the soil. Values of K_d are typically reported as K_{oc} , where K_{oc} is the distribution coefficient normalized to organic carbon.

ALAM: The "radioactive" decay factor of the contaminant in the saturated medium. The rates can be altered to additionally reflect biodegradation and volatilization where information is available. Rates are 1/days.

ALFA: Similar to ALAM, but represents the rate of decay of the source strength. Specify ALFA=0. for constant source strength. An example of the modeling process is illustrated in the following figures. A user-friendly menu-driven preprocessor has been created for ODAST. This preprocessor allows a user to create and/or edit data files. The preprocessor can be executed by invoking the "Input Data" option in the top menu of the

shell screen. Figure 16 shows the help file for the ODAST preprocessor. Users can obtain documentation about the input format and detailed explanation of variables. Figures 17 through 21 show the sequence of screens during the modeling process. The messages displayed on the screen should guide the users to enter proper responses.

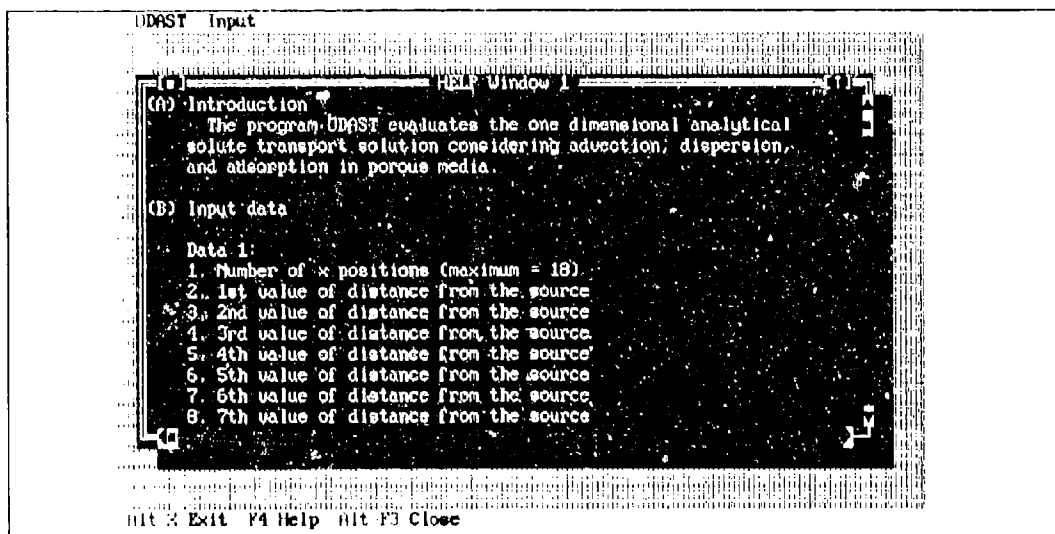


Figure 16. Help file for ODASt Preprocessor

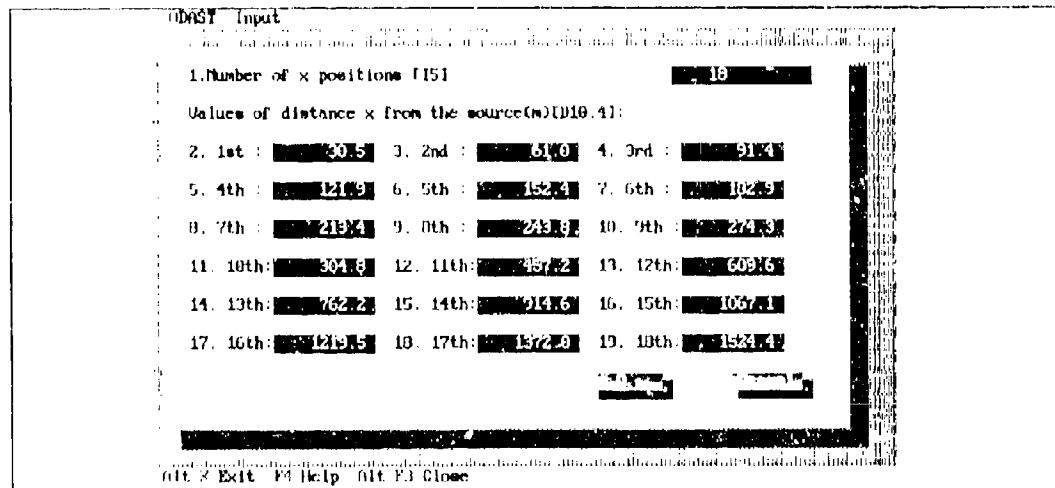


Figure 17. Input data set 1 for ODASt

ODAST Input

1. Dispersion coefficient in m ² /day [D10.4]	5.09
2. Seepage velocity in m/day [D10.4]	0.0835
3. Retardation factor [D10.4]	4.5
4. Period of solute recharge in years [D10.4]	36.
5. Solute decay constant [D10.4]	0.
6. Source decay constant [D10.4]	0.

Alt X Exit F4 Help Alt F3 Close

Figure 18. Input data set 3 for ODAST

ENTER CONCENTRATION C0: 1.0

ENTER NAME OF CONTAMINANT AND
UNIT OF CONCENTRATION e.g. TCE (mg/l): TCE

ENTER SITE NAME: H111

Figure 19. Screen for Entering Contaminant Name

Screen output options include graphing the breakthrough curve (Figure 20) or viewing the actual output file printed by the transport model program (Figure 21). Both of these screen options can be sent to the printer also using built-in utilities.

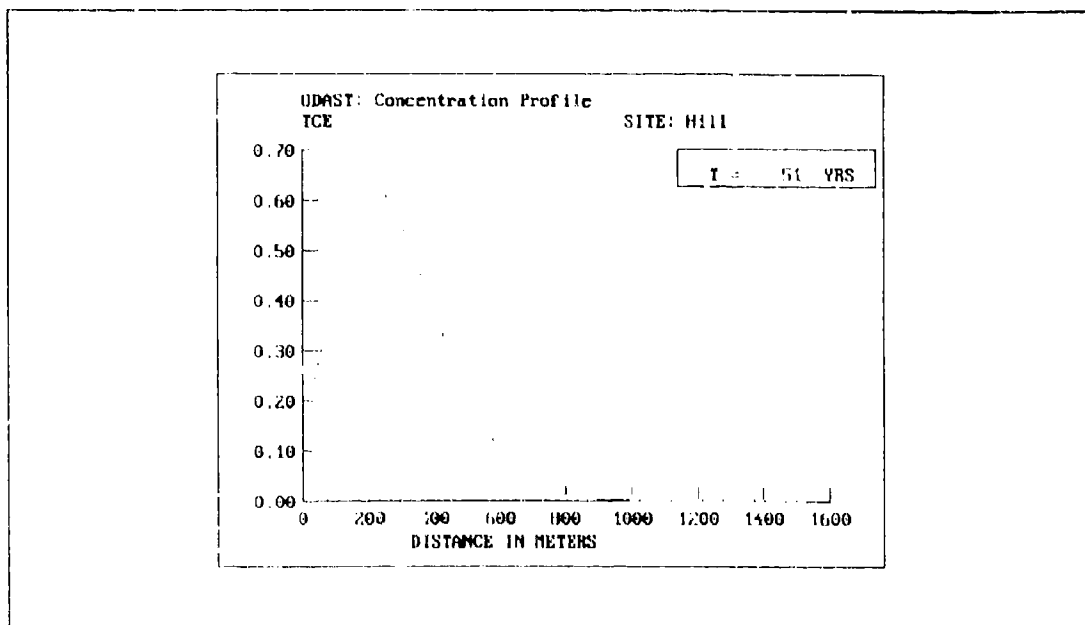


Figure 20. Graphical output from ODAST

Utilities Input Data Run PostODAST View Files						
model.out						
SOURCE CONCENTRATION CO = 1.00						
CONCENTRATION (C) FOR						
U= .03 D= 5.09 R=4.5 LAMBDA= .000 ALPHA= .000 TO= 36.0						
T(YEARS)	X= 31	X= 61	X= 91	X= 122	X= 152	X= 183
51.0	2373D+00	3206D+00	4117D+00	5002D+00	5637D+00	6044D+00
CONCENTRATION (C) FOR						
U= .00 D= 5.09 R=4.5 LAMBDA= .000 ALPHA= .000 TO= 36.0						
T(YEARS)	X= 213	X= 244	X= 274	X= 305	X= 457	X= 610
51.0	6205D+00	6135D+00	5870D+00	5459D+00	2738D+00	8733D-01
Alt-X Exit F1 Help Alt <char> Menu						

Figure 21. Option for viewing the output file

2. TDAST

The model TDAST evaluates the two-dimensional solute transport case with an analytical solution, considering convection, dispersion, decay and adsorption in porous media (Javandel et al., 1985). The idealized conception of the model is related to that of ODAST, but covers another important class of cases. As with TDAST, we assume conditions of steady-state, uniform flow in a confined aquifer. The source is again assumed to be fully penetrating, but in this case is of finite lateral extent (normal to flow), as in the case of a fully penetrating ditch of finite length. Thus TDAST is applicable in conditions similar to those applicable for ODAST, except that here the observation point is far enough from the source boundary so that the effects of the source edge and transverse dispersion must be taken into account in the approximation. By using the same techniques as described above for ODAST, TDAST may be applied to constant areal waste sources. In such a case, ODAST would be accurate for analysis near to the center of the source edge, while TDAST could be used for such a location and also locations nearer to the source edge, and locations further away from the source boundary. In general, the numerical stability and speed of ODAST make that solution preferable where applicable. TDAST is also useful for analysis of contamination resulting from smaller sources.

The same general **limitations** apply to TDAST as apply to ODAST, except that the effects of lateral source geometry and transverse diffusion are explicitly considered. That is, the approximations of full penetration (vertical mixing) and uniform, steady state flow must also be met here. TDAST also assumes that the source is aligned normal to the regional flow, although the solution could readily be altered to take into account other geometries. An important practical limitation of the present version of TDAST arises from its use of a numerical technique to evaluate an integral. Presently TDAST uses a Gauss-Legendre polynomial method for this evaluation, making use of the same subroutine employed in the models EPASF and EPAGW. The number of terms in the polynomial evaluation may be set by the user, up to a certain limit. The solution routine begins with a lower number of terms and increments the number until the solutions converge (within 1%), or the limit is reached. Under certain conditions adequate convergence cannot be achieved within the limits available in the numerical integration scheme, which will result in the display of a warning message. In general, lack of convergence will be encountered when the ratio of Vt/X becomes much greater than 1 (where V is velocity, t is time and X is distance). This means that TDAST provides accurate calculation of the time period during which concentration increases at a given point, as the plume breakthrough occurs, but loses accuracy at a given point as time increases past breakthrough, resulting in underestimation of concentrations. However, this is merely an inconvenience for analysis, as the solution should approach a steady-state concentration before numerical instability overwhelms the solution. The user should thus fine-tune the application to avoid this problem. This can be done for the desired time step by eliminating those observation points that are well behind the breakthrough curve of the plume.

TDAST shares a similar preprocessor to that of ODAST. Figure 22 shows a typical screen from the TDAST preprocessor. The data-input format is thus essentially the same as that for ODAST, described above, with the addition of the following variables:

NUMY: Number of Y positions in the grid. Observations will be calculated at all combinations of NUMX, NUMY and NUMT.

NNS: This sets the accuracy of the numerical integration scheme used by TDAST, by choosing the degree of the polynomial for the Gauss-Legendre method. NNS selects the nth digit from (4, 5, 6, 10, 15, 20, 30, 40, 50, 60, 104, 256). Increasing NNS improves accuracy but decreases speed. NNS=8 seems to provide a good compromise value with which to start, but may be changed at will. If convergence warnings appear on screen during run time the user should try increasing the value of NNS.

DT: Transverse dispersion coefficient.

A: Half-length of the source, being 1/2 of the lateral extent of the source normal to the direction of flow.

TDAST Input

1. Longitudinal dispersion coeff. (m^2/d) [E10.4]	1.
2. Transverse dispersion coeff. (m^2/d) [E10.4]	1.
3. Pore water velocity (m/d) [E10.4]	1.
4. Half length of source (m) [E10.4]	50.
5. Radioactive decay factor (1/day) [E10.3]	0.
6. Retardation factor [E10.3]	1.
7. Decay factor of the source (1/day) [E10.3]	0.

OK Cancel

Alt-X Exit F4 Help Alt-F3 Close

Figure 22. Input data set 6 for TDAST

3. PLUM2D

The model Plume 2D (van der Heijde, 1985), here referred to as PLUM2D, is an analytical model for calculation of the tracer concentration distribution in a homogeneous, non-leaky confined aquifer with uniform regional flow. The solution method is based on the Hantush Well-function, in which the Well function flow solution for a leaky confined aquifer is applied by analogy to account for transport and dispersion in a non-leaky confined aquifer. Source strengths are assumed constant, but the solute may be subject to adsorption and radioactive type decay in the porous medium.

An important advantage of this method is that it can readily treat multiple point sources, which sources may have been operational for differing amounts of time. This enables PLUM2D to treat certain situations that cannot be handled by other analytical methods. The solution is based on an idealized situation, in which solute is introduced into a fully homogeneous confined aquifer through one or more fully penetrating wells in the presence of regional two-dimensional, horizontal ground water flow. The injection rate from these wells is considered to be sufficiently small that it does not alter the regional flow pattern. Thus the model is most applicable to the case of injection wells with relatively low injection rates. However, PLUM2D can also provide a reasonable approximation for other situations. That is, surface sources can be modeled as fully penetrating sources if the assumption is made that the solute is fully mixed in the vertical direction soon after its introduction into the aquifer. Further, the solution method is approximately appropriate for use in a surficial aquifer, when the saturated thickness is relatively constant, and the leaching rate from the sources is of a small enough magnitude such that it does not affect the regional flow regime through mounding.

In incorporating the model into the system we have provided a complete preprocessor and equipped the model for Monte Carlo simulation. To account for the correlation of the various parameters controlling the regional flow regime these are generated from simpler, underlying variables (see discussion of EPAGW for more details). However, user option is also provided in the Monte Carlo mode for direct input of hydraulic conductivity and dispersion values.

As with many of the other two-dimensional analytical models incorporated into the system, use of PLUM2D is **limited** to cases where it is reasonable to model the aquifer as if it were a confined aquifer with fully penetrating sources. These sources are treated as point sources, and thus the model is applicable to areal sources only where these can be treated as clusters of point sources. The model further assumes that source strength is constant, once initiated, and cannot handle situations in which the strength of the source is decaying over time.

As with most models in the system, we have provided a standard format preprocessor for PLUM2D. The user is provided with an option to specify input in either metric units [m, day] or English units [U.S. gallon, ft., day]. Data input is as follows:

UNITS: User option to select English or metric units.

TITLE: Title to be used for output.

NPTS: Number of solute injection wells specified, or other sources that can be approximated as injection wells. Up to 10 may be used in the present configuration of the model.

NOBS: Number of observation points for Monte Carlo simulation (up to 5). These are the points at which cumulative concentration frequencies will be calculated, and are in addition to the gridded calculation of concentration. For deterministic mode this variable is not needed.

NX: Grid dimension for calculation, number of nodes in x-direction. As this is an analytical solution, for Monte Carlo simulation a very sparse grid may be specified if interest is in only the frequency of concentrations at the observation points, rather than plume development. Specifying a sparse grid will greatly speed execution. The X axis is assumed to be coincident with the direction of regional flow. NX can range from 2 to 20.

NY: Grid dimension for calculation, number of nodes in y-direction. Range 2-20.

IRAD: User option to include radioactive decay (1=yes, 0=no). As in other models, decay processes such as hydrolysis can often be modeled as radioactive decay, if an effective "half-life" can be established. PLUM2D does not include the ability to model hydrolysis based on pH, with pH specified as a random variable.

MODE: User option for Monte Carlo simulation. Set Mode=1 to generate K from underlying variables of particle size and gradient, set Mode=2 to estimate K as a log-normal distribution independent of particle size.

XS: X-coordinate of origin of grid, in appropriate units. Range 0. to 5000.

YS: Y-coordinate of origin of grid, in appropriate units. Range 0. to 5000.

DXOB: Grid spacing (interval) in the X direction. PLUM2D thus specifies an evenly spaced grid.

DYOB: Grid spacing in the Y direction, may differ from DXOB and is typically smaller than DXOB.

V: Average Darcy velocity of uniform regional flow, in the appropriate units, coincident with x axis. Required in deterministic mode only. In Monte Carlo mode V is generated from underlying hydrogeologic variables.

M: Average aquifer saturated thickness, which is assumed constant.

P: Effective porosity(as a fraction). Required in deterministic mode only.

L: Longitudinal dispersivity, in units of length. Note that this model requires input of dispersivity, rather than dispersion coefficients.

T: Transverse dispersivity, in units of length.

RD: Retardation coefficient. $RD = V/V_c$, where V is the regional velocity and V_c the apparent velocity of the contaminant. Thus RD must be ≥ 1 . Enter RD=1. for no retardation.

HL: If radioactive decay has been specified, enter half-life, in years.

The next eight variables are required only in the Monte Carlo mode:

ITER: Number of iterations (runs) for Monte Carlo mode. ITER is recommended to be set to at least 500 to provide adequate definition of the frequency histogram. However, the user will usually wish to first test model performance by setting ITER to a smaller number.

CVI: Coefficient of variation of leachate (injection) concentrations, where the coefficient of variation is the standard deviation divided by the mean. The injection concentrations are modeled as a normal process.

TH(1), TH(2): The mean particle size is modeled as a log-10 uniform process, measured in centimeters. TH(1) is the maximum of the range of the mean, while TH(2) is the minimum. Thus TH(2) must be \leq TH(1).

GR(1),GR(2),GR(3): The hydraulic gradient is modeled as a triangular distribution, in which GR(1) is the most likely value, GR(2) the minimum value and GR(3) the maximum value. The range of GR is restricted to $1.0E-5$ to 0.1, expressed as length per length.

CVD: Coefficient of variation for dispersivities, applied to both L and T.

CVLNQ: Coefficient of variation of leaching (injection) rates. If the HELP model has been applied to this site the observed coefficient of variation from the HELP results will be reported.

DKLN: Required only if MODE is set to 2, and hydraulic conductivities are to be independently generated. DKLN is then the mean of the natural log of hydraulic conductivity, in cm/sec.

DKLNV: Standard deviation of mean LN hydraulic conductivity. Required only if MODE is set to 2.

DATA SET 1: OBSERVATION POINTS. Required only in Monte Carlo mode. For each observation point specified by NOBS the user must enter the x and y grid index (IXOBS and IYOBS).

DATA SET 2. INJECTION WELLS. For each injection well, or source modeled as an injection well, the user must enter the following values:

X: x grid coordinate of the source.

Y: y grid coordinate of the source.

Q: injection rate of the source, specified as gpd or m^3/d , as chosen by UNITS.

C: solute concentration of injection, as mg/l or ppm.

TIME: time since start of injection (operation) of this source, in days.

Figure 23 is the main menu for PLUM2D. To choose an option, simply type the number of the option and press the enter or return key. Figure 24 is the menu that allows one to edit groups of data. As each group of data is edited, variable names and values appear on the screen. Figure 25 is an example of graphical output.

```
#10          PLUM2D PREPROCESSOR MAIN MENU

Data preparation options for Plume-2D
-----
Prepare a new data set . . . . . 1
Edit current data set . . . . . 2
Input data set from site file . . . 3
Save data set for future use . . . 4
Show HELP screen . . . . . 5
Exit preprocessor and run model. . . 6
Terminate session . . . . . 7

ENTER SELECTION:
```

Figure 23. Main menu for PLUM2D

```

#2  PLUM2D                      EDIT SCREEN SELECTION
Select a screen you want to edit or review, and enter its number.

      cards                      number
-----
card 1. Title . . . . . 1
card 2. Control card 1. . . . . 2
card 3. Control card 2 (grid) . . . . 3
card 4. Hydrogeology card . . . . . 4
card 5. Monte Carlo controls. . . . . 5
data set 1. Observation points. . . . . 6
data set 2. Injection wells . . . . . 7
      All cards in sequence . . . . . 8

Selection (RETURN to exit):

```

Figure 24. EDIT screen selection for PLUM2D

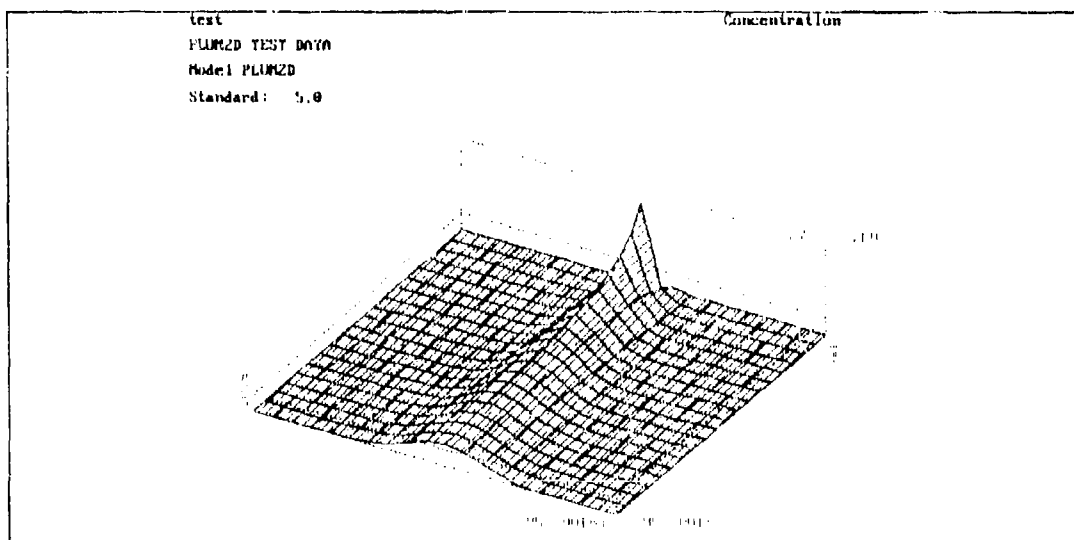


Figure 25. Graphical output from PLUM2D

4. DUPVG

The above two analytical models are limited in their use to situations in which the aquifer can be modeled as approximately equivalent to a confined aquifer. Serious problems with this assumption arise when leaching from a source is of sufficient volume relative to regional flow to create a significant radial flow component. The source then serves not only to introduce contamination, but also alters the flow regime, and the aquifer will possess a moving free surface. The significance of such effects is estimated in the CHOICE algorithm by a preliminary calculation of ground water mounding resulting from the source. Where significant movement of the free surface is expected few analytical solutions are available. Model DUPVG provides a solution for a particular class of these problems (Volker and Guvanasen, 1987; Guvanasen and Volker, 1982).

DUPVG is a two-dimensional model in the X-Z plane, considering the longitudinal and vertical distribution of the contaminant. The geometry is thus an extension of the one-dimensional case. The source is represented as an infinitely long recharge basin of a fixed width which contributes a constant rate of recharge to the aquifer. The aquifer is assumed to be symmetrical in X about this source, and bounded by a constant head drain at a fixed distance, and there is assumed to be no pre-existing regional flow pattern. This enables the calculation of an approximate velocity distribution within the saturated zone, and thus contaminant distribution. The assumption of an infinitely long recharge basin implies that this model will be appropriate when the point of observation is sufficiently close to the source so that the effect of finite lateral extent of the source is unimportant, as in the application of ODAST. DUPVG is thus particularly important for estimation of plume development near to a large areal source which contributes significantly to the flow regime, such as surface irrigation systems.

It should be reemphasized that the only flow considered by DUPVG is that induced by the source. Thus dispersion is the only mechanism for dilution of the source concentration. As decay is not considered, this means that if DUPVG is run for a sufficiently long time it will eventually "flood out" the aquifer with water at the source concentration. It is thus not particularly useful to run the model for predictions at a given distance if the time involved is sufficient so that water at source concentration has fully occupied this point - for in this case the prediction is merely that the concentration is equal to the source concentration. A rough estimate of the occurrence of this phenomenon is when:

$$\frac{QAt}{7.48 snR} > x \quad (2)$$

where Q is the areal leaching rate in gallons per day per square foot, A is the half-width of the source along the direction of flow, in feet, t is time in days, s is the initial saturated thickness, in feet, n is porosity, R is retardation coefficient (v/v_r) and x is distance to the observation point in feet. Where this inequality holds the controlling criteria for

concentration predictions will be the determination of Q , and any vadose zone attenuation of contaminant load. The analyst may also need to consider whether any processes of decay or dilution by regional flow, which cannot be considered by this model, may have a significant effect.

In order to derive the analytical solution a number of important simplifying assumptions were made, and the user should be aware of the implications of these assumptions. The solution method first assumes that the rise of the free surface is substantially less than the initial saturated thickness of the aquifer (tests of this condition are made in the CHOICE algorithm). Based on this premise it is assumed that:

(1) The unsteady free surface can be approximately described by a streamline, which implies that the flow pattern is equivalent to the confined case, but with an a priori unknown upper boundary.

(2) Near the source, streamline and equipotential functions change little with time, so that the transient velocity can be described by a steady state distribution modified by a simple time function.

(3) Further away from the source the velocity field is essentially horizontal and its spatial variation is negligible.

These conditions require that the slope of the free surface is relatively small, and that the distance to the constant head drain is sufficiently large so that equipotential lines at the downstream end are vertical. The final solution uses an approximation that is equivalent to the case where the distance to constant head goes to infinity, although the near source velocities are first computed using a finite value of this distance. In any case, the solution method will be accurate only when the constant head boundary is relatively far away from the source. Further, constant head boundaries must be assumed to be distributed symmetrically about the source axis.

The approximate solution employed for the transport equation (S1) is based on the assumption that the distance to constant head can be extended to infinity. However, the velocity distribution is first calculated without this approximation. Thus the solution method should provide an accurate estimation of the average position of the front. However, when the constant head boundary is closer to the source the vertical distribution of concentrations may not be accurate.

Other important limitations are obvious from the nature of the solution. The method cannot take into account any regional flow other than that induced by the source. Further, the method treats only conservative substances, which may be retarded but are not subject to decay.

The preprocessor for DUPVG shares the similar format as that of ODAST and

TDAST, and information given in the discussion of ODAST is relevant to the DUPVG input file. The data to be input are as follows:

NUMX: Number of points modeled in the X direction, which establishes the 1-dimensional grid.

NUMZ: Number of points modeled in the vertical, Z direction, counting downward from the top of the saturated zone.

NUMT: Number of time steps for calculation.

NNS: The solution requires numerical integration of one simple time derivative. NNS sets the accuracy of the numerical integration scheme by choosing the degree of the polynomial for the Gauss-Legendre method. NNS selects the nth digit from (4, 5, 6, 10, 15, 20, 30, 40, 50, 60, 104, 256). Increasing NNS improves accuracy but decreases speed. NNS=8 seems to provide a good compromise value, but may be changed at will.

Q: leaching rate from source expressed as gal./ft²-d. If the HELP model has been run for this site, the values obtained will be reported here. In DUPVG the source is conceived as a basin of infinite horizontal extent and finite width.

POR: Total porosity of the medium.

B: Thickness of saturated layer (initial thickness). This is used to calculate the initial mixed concentration beneath the source.

DL, DT: Dispersion coefficients.

A: For DUPVG, this measures the effective width of the "infinite" source along the X (flow) axis. This is properly the distance from the edge of the source to a flow divide. As the geometry is assumed symmetrical this is equivalent to half of the width of the source in X.

R: retardation coefficient, $= v/v_c$, where v is the velocity of the regional flow and v_c the apparent velocity of the contaminant.

SST: Mean initial source strength, as ppm.

FC: Field capacity (fraction). Porosity $= P_e + FC$, where P_e is the effective porosity.

PKW: In DUPVG, an initial estimate of K is required.

AHW: Determination of the slope of the free surface requires specification of distance to a constant head boundary, assumed to be symmetrical about the source. Note that for the approximation method used in the solution accuracy decreases as the observation point becomes nearer to the constant head boundary.

ATTEN: Fraction of the solute remaining after vadose zone attenuation. If the HELP model has been run a conservative estimate of ATTEN can be calculated automatically. This calculation assumes that the substance proceeds downward through the unsaturated zone at pulses equal to the saturated hydraulic conductivity of that zone, subject to retardation, and thus provides a very conservative estimate of residence time.

5. EPAGW

The basic model employed here was developed by the EPA for analysis of restrictions on land based disposal, and is documented U.S.E.P.A. (1986). The EPA approach is to model the transport of a given substance, subject to hydrolysis and retardation, determining a downflow dilution factor which is used to back-calculate an allowable concentration of the substance in a landfill, given a down-flow standard level. To do this, Monte Carlo simulation is undertaken over all the relevant hydrogeological variables, using a national data set, allowing the formation of generalized regulatory standards for allowable concentrations within the landfill. The method is carefully designed to account for the correlation among simulated parameter values. The transport model employed is Sudicky et al.'s (1983) 3-D steady-state solution, using Gaussian quadrature to solve the integral. We have modified this method in a number of ways. First, if we assume that the site characteristics are known, or can be specified by distributions, the method is readily inverted, so that the "dilution" factor is used to predict downstream concentrations from a specified source, using the same Monte Carlo analysis. Secondly, instead of using a national data base for the hydrogeologic parameters, one of several data bases can be selected that reflects the characteristics of a specific region within North Carolina. The selected data base can then be modified in accordance with any available site-specific data. The method thus becomes appropriate for an analysis of contamination risk in a situation in which little is known about the specific hydrogeology of a site. The objective is then to simulate the expected risk over the range of hydrogeological conditions that are expected to apply for the specific region in which the site is located.

The source in the EPAGW model is assumed to be distributed as a Gaussian source. The source is thus areal, but concentrated towards a central point. This makes the model particularly applicable to landfills. However, it may be inappropriate for large scale areal sources, such as surface irrigation of wastes, in which contaminant input is relatively uniform across the source area.

EPAGW represents a complete and coherent Monte Carlo approach to contaminant risk analysis under uncertainty. It is thus the model of choice for preliminary analysis of risk in situations in which little site specific data is available on flow regime and hydrogeology, given that a Gaussian representation of source distribution is appropriate. The model development assumes that the direction of flow from the source is not accurately known. Analysis is thus made at a specified distance along the (unknown) main axis of flow. Equivalently the model may be applied to analysis along an explicitly known axis of flow.

EPAGW contains detailed routines for calculation of chemistry dependent hydrolysis of contaminants. It also considers the effects of vertical mixing. The model will thus also be useful for analysis in some situations where there is substantial knowledge regarding the flow regime, but the analysis requires consideration of partial penetration and/or complex hydrolysis reactions. This is especially useful for analysis of certain organic constituents with pH dependent hydrolysis rates.

EPAGW provides a highly flexible method for analysis. However, it can only be applied in the Monte Carlo mode. Further, solution is provided only at a point along the axis of flow at the surface of the aquifer. A steady-state concentration only is calculated, so that EPAGW cannot be used to calculate time history of contamination. From the nature of the solution the model will not be appropriate for large uniform areal sources, such as land applications. The usual assumptions of steady-state, uniform flow apply here, and the model will not be appropriate for sources that contribute a volume of fluid sufficient to significantly alter the flow regime.

Data input for EPAGW consists of two phases. The first phase concerns the parameters controlling site hydrogeology. To initiate this phase for a new site the user should first load a default regional data set from the list provided. Even where an appropriate regional data set is not available one should be loaded to guide input, then modified as needed.

Development of regional data sets is still in progress, but limited by available information. For regulatory analysis it will most commonly be the surficial aquifer that is of interest. These can be conveniently grouped according to the nature of the surface soil. The specification of the underlying hydrogeologic parameter distributions and their probability parameters is designed to allow a maximum of flexibility in selection. First, a regional data base with assumed distributions and metaparameters is selected. Where no additional site data or user knowledge is available, simulation may proceed with these unaltered distributions and values. This will provide an estimate of contamination risk based on the average characteristics of the area, and so should be modified to reflect any known differences of a specific site location from the average characteristics of the area. However, any parameter distribution may be altered in one or more of the following ways:

1. Respecify parameter distribution metaparameters.
2. Automatically update regional data by combination with site data.
3. Respecify parameter distribution type.

Where the user feels that a given parameter is known with considerable accuracy this may be indicated by specifying the distribution as a tightly restricted uniform or triangular distribution.

The types of distributions that may be specified for the various parameters are identified as follows:

0. No distribution has yet been specified. This must be replaced before running the model.

1. Triangular distribution. The user must specify most likely, minimum and maximum values for the distribution. The triangular distribution is an ad hoc, empirical distribution which takes a triangular shape. This can be used to readily approximate various peaked but skewed distributions.

2. Uniform distribution. The user must specify the minimum and maximum of the range.

3. Log 10 Uniform distribution, in which the log values are uniformly distributed. The user must specify the UNTRANSFORMED minimum and maximum values of the range.

4. Normal distribution. The user must specify the mean and standard deviation.

5. Log-normal distribution, in which the log values are normally distributed. The user must specify the mean and standard deviation of the log transformed values.

6. Exponential distribution, in which the mean is equal to the standard deviation. The user must specify this single value.

7. Table-specified distribution. This is available in certain cases only.

Each of the pre-specified regional data sets will describe each of the parameter distributions by one of the above distributions. However, these may vary from data set to data set. For this phase of input, distributions must be specified on the following parameters:

DIAM: mean particle diameter (cm). Note that the specification is of the distribution of the mean, not the full range of particle diameters encountered.

GRAD: gradient of the water table (length per length).

FOC: organic carbon fraction of aquifer medium. This is an important factor in the chemical analysis of the fate of certain organic constituents.

PH: pH of groundwater.

T: groundwater temperature (Centigrade).

TH: thickness of the saturated zone (meters).

H: leachate initial penetration depth into the saturated zone (meters). This specifies vertical mixing beneath the site. Because of constraints in the solution method H must be equal to at least 2 meters.

QC: leaching rate distribution for engineered (lined) facilities.

QD: leaching rate distribution for non-engineered facilities (Default is table specified; for direct input use m/yr). If the HELP model has been applied to the site the leaching rates estimated from this model may be loaded to replace both the QC and QD values.

Phase one thus requires specification of the general characteristics of the aquifer. Phase two of data input requires information on the site engineering and the contaminant of interest. The following data are required:

CLM: mean leachate concentration, in mg/l (ppm).

CLS: standard deviation of leachate concentration mean.

DKA0: hydrolysis rate for the substance under acid conditions, 1/[molar-year]. EPAGW simulates the lumped degradation constant, K, based on pH, DKA0, DKB0 and DKN0. Values of hydrolysis rate must be converted to years⁻¹ for input to EPAGW.

DKB0: base catalyzed hydrolysis rate, 1/[molar-year].

DKN0: neutral catalyzed hydrolysis rate, 1/year.

DKOW: \log_{10} octanol/water partition coefficient for contaminant, describing the constituent's solubility. The actual value will be dependent on the organic carbon content and available surface area of the soil. If this value is not directly known it may be estimated from:

$$DKOW = 5.0 - 0.67 (\log_{10} (S_w)) \quad (3)$$

where S_w = solubility in water. EPAGW also uses DKOW to estimate the adsorption coefficient of the constituent, using the approximate relationship:

$$\log_{10} K_{oc} = 1.029 (\log_{10} K_{ow}) - 0.18 \quad (4)$$

Note that this relationship may not be valid for polar constituents.

ATTN: a factor which specifies the fraction of solute remaining after passage through the unsaturated zone beneath the landfill. If the HELP model has been applied to this site a conservative value of ATTN may be calculated automatically from the HELP output. This is calculated in the same manner as for the model ODAST.

NPROB: number of Monte Carlo runs. A minimum of 500 is recommended for adequate definition of the cumulative frequency. However, the user will usually wish to test model performance by first trying a smaller number of runs. The value of NPROB is not saved with the data set, but defaults to 500, and thus may need to be respecified for each run.

AW: surface area of landfill, in square meters.

TR: reference temperature for the chemical rate constants, in degrees C (these are usually specified at 25° C).

XX: distance from the edge of the disposal area to the observation point, along the flow axis (meters). The exact value of XX is ambiguous for large areal sites.

Leaching Rate Distribution: Calculated from HELP model, or from table, where

C: table for engineered facilities

D: table for nonengineered landfills.

6. EPASF

The EPA surface water model (EPASF) was designed to assess impacts of waste disposal sites on surface waters (with hazard associated with human use of contaminated surface waters or consumption of fish from contaminated surface waters) in a manner analogous to the EPAGW model. Here, however, at least two stages must be considered: transport from the landfill via groundwater, and entry into and dilution in the stream. As with the EPAGW model, we have modified this model to provide risk assessment from a given landfill, and have likewise added a preprocessor. EPASF and EPAGW can share essentially the same input data set, with a few additions.

EPASF estimates groundwater contaminant transport to the stream using either a one dimensional or a three dimensional solution, and with or without consideration of dispersion. In the three dimensional case the transport solution is the same as that used in EPAGW. Note that lateral dispersion of the contaminant plume affects the concentration, but not the total mass loading to the stream. As EPASF provides only a very generalized approximation of the transport process analysis without dispersion will often be adequate for a first estimate.

EPASF provides only a preliminary estimate of impacts in surface waters. However, modeling the interaction of groundwater and surface water often presents formidable difficulties, so that one is forced, by default, to rely on a model such as EPASF for a preliminary estimate of risk. It should be remembered however that EPASF presents only a preliminary estimate. If contamination problems are suggested by application of EPASF the user may then need to attempt more sophisticated analysis.

EPASF uses essentially the same data input format as EPAGW, and can share the same data sets. However, distributions for two additional parameters must be specified when characterizing the hydrogeology. These are:

FOCS: organic carbon fraction of suspended sediment in the stream.

FL: lipid fraction of fish biomass. This is needed only where human impact is assessed via consumption of fish from the stream. The lipid fraction is used to assess bioconcentration of certain lipophilic organic constituents.

Input of the site parameters is very similar to that for EPAGW, but possesses a few differences, including slight alterations in variable names. The site data input for EPASF are defined as follows:

DIMNSN: Dimension of problem; the groundwater transport phase may be run using a one dimensional or three dimensional solution. The one dimensional solution of course results in much quicker execution of the model.

DSPRSN: Effects of dispersion may be included (1) or omitted (0).

X: distance from landfill edge to the stream, in meters.

CLM: leachate concentration, mg/L (ppm).

CLS: standard deviation of leachate concentration.

LKOW: log octanol / water partition coefficient for contaminant species.

KHA0: acid-catalyzed hydrolysis rate, 1/[molar-year].

KHB0: base-catalyzed hydrolysis rate, 1/[molar-year].

KHN0: neutral pathway hydrolysis rate, 1/year.

TREF: reference temperature for hydrolysis rates, degrees C (usually at 25° C).

NUMRNS: number of Monte Carlo runs. At least 500 runs are recommended, and in most cases this model is moderately fast.

AW: area of waste site, square meters.

AS: area of watershed above point of impact, in square miles. This factor is used in the determination of in-stream dilution.

Leachate distribution: flux of leachate from landfill, in m/yr. Choices: subtitle C (engineered), subtitle D (non engineered). As in EPAGW these values may be replaced by rates calculated by the HELP model.

ATTN: factor specifies the fraction of solute remaining after passage through the unsaturated zone beneath the landfill. If the HELP model has been applied to this site a conservative value of ATTN may be calculated automatically from the HELP output.

7. LT RD

LTIRD calculates the concentration of a particular solute in radial flow (Javandel et al., 1984), using a semianalytical solution originally written by Moench and Ogata (1981). This model is included for the explicit purpose of treating purely radial flow situations, in which regional flow is not present. The idealized situation treated by the model considers a confined aquifer of constant thickness which is recharged through a fully penetrating well at a constant rate. The model considers steady-state plane radial flow only.

As with other solutions for confined aquifers, LTIRD is applicable as an approximation to unconfined aquifers in cases where mounding is sufficiently small so that the streamlines remain approximately parallel. LTIRD can also be used to treat surface inputs if the assumption can be made that the solute is vertically mixed in the aquifer soon after introduction.

LTIRD has a rather **limited range** of applications in the advisory system. There is no consideration of regional flow, so this model should be used only when the radial flow from recharge dominates, but, in the case of a surficial unconfined aquifer, the rate of recharge is also sufficiently small so that the assumption of a confined aquifer is approximately valid. Use of the model is also limited by the fact that it does not include decay or retardation, and the fact that it assumes steady-state plane radial flow. The source is modeled as a well, so that the model is not appropriate to areal sources.

Data input for LTIRD is quite simple. The following are required, in any consistent units:

NUMR: Number of radiuses at which to calculate concentrations.

NUMT: Number of time steps to calculate.

RDW: Radius of the well, or source approximated as a well.

R (1 to NUMR): Radial distances at which calculations are made.

T (1 to NUMT): Times for calculation.

ALPHA: Dispersivity.

Q: rate of recharge.

B: Saturated thickness of aquifer.

N: Porosity of aquifer.

C0: Concentration of solute in recharge.

8. RESSQ

RESSQ is a program for semianalytical calculation of contaminant transport (Javandel et al., 1985). The model calculates two-dimensional transport by advection and adsorption (no dispersion or diffusion) in a homogeneous, isotropic confined aquifer of uniform thickness when regional flow, sources, and sinks create a steady-state flow field.

Recharge wells and ponds act as sources and pumping wells act as sinks. The solution proceeds by calculating the streamline pattern in the aquifer and the location of contaminant fronts around sources at various times. RESSQ can thus be applied to a large variety of complex flow situations that can not be handled by analytical solutions.

Because the method is limited by neglecting dispersion, RESSQ, as other semianalytical methods, is most appropriate for preliminary analysis of the extent of probable contamination in a complex flow regime. If the semianalytical method does suggest a contamination problem at the perimeter of compliance the user may then need to apply a more complex numerical model. Because it is a preliminary analysis tool, RESSQ is provided only in a deterministic mode. An example application is provided in subsection III(G).

The most obvious limitations of RESSQ are its neglect of dispersion and decay. Other limitations of the method are similar to those that apply to most two dimensional steady state analytical solutions. RESSQ requires that the medium is homogeneous and isotropic, with steady state uniform regional flow. Thus the method is not applicable when the medium is distinctly heterogeneous or anisotropic. Further, the method is not directly applicable to transient problems.

A more subtle limitation is due to the assumption made in the model that a steady state flow field exists. This implies that the sum of flow rates from all the injection wells should be equal to the sum of the flow rates from all the production wells. In practice, RESSQ can be applied to situations where these sums are not equal, if analysis is made at sufficiently large values of time so that quasi-steady flow prevails (see below). However, if attempts are made to apply the model to shorter time periods where the two sums are widely different bizarre results may occur. Note that this problem is avoided if a constant head boundary is specified through the use of image wells, in which case the two sums will be by definition equal.

The solution method used in the model is based on the assumptions of a uniform, confined aquifer. Application to a surficial aquifer is thus valid only when conditions in the surficial aquifer approximate those of a confined aquifer. For a preliminary analysis of contaminant risk this is appropriate when the surficial aquifer does not show distinct seasonal variability, and the input from sources does not result in substantial mounding. The latter condition should be adequately met in situations for which the Dupuit approximations hold. In addition, and like most available two-dimensional analytical solutions, RESSQ assumes that sources fully penetrate the aquifer. This is equivalent to assuming that the contaminant loading from a source instantaneously displaces the pre-existing water throughout a vertical column of the aquifer. Note that RESSQ provides a sharp front approximation, and cannot account for mixing of the flow from a source with the water in the aquifer. Instead, the source flow displaces the water in the aquifer, without mixing. For a source that is not actually fully penetrating this approximation is obviously more valid for a thin saturated layer. However, an overly thin saturated layer

is likely to result in violation of the confined aquifer approximation. The practical result is that RESSQ, when applied to a surficial aquifer with a non-penetrating source, is likely to provide inappropriate concentration results in the region close to the source, but more accurate results further away from the source.

Attempts to apply RESSQ to surficial sources which do not fully penetrate the aquifer are considerably complicated by the necessary assumption that no mixing occurs. This may result in overestimation of the concentration resulting from a source. This is a particular problem when the rate of regional flow is significantly large in relation to the rate of recharge from the source. In such cases the positions of contaminant fronts can still be calculated, but the concentration within these fronts cannot be interpreted as equal to the source concentration. In general, RESSQ is recommended for approximate application to surficial sources only in cases where the flow from such sources is of sufficient volume to overwhelm the regional flow in the neighborhood of the source and a radial flow pattern is established. In sum, it should be emphasized that RESSQ is best thought of as a preliminary analysis tool. Despite the many limitations expressed above it provides a very powerful tool for preliminary analysis of complex flow situations.

Appropriate use of RESSQ is somewhat of an art, and will require practice on the part of the user to obtain adequate results. This is because the model calculates concentration front positions on the basis of a finite number of streamlines. The results observed are thus to a degree sensitive to the number of streamlines modeled, and the starting angle of the first streamline leaving each source. The user may need to experiment with these values to obtain the desired results.

By proper formulation of the input data RESSQ can be used to model a wide variety of situations. The following suggestions for data input are taken from Javandel et al. (1984):

(1) If the total flow rate from all injection wells does not equal the total flow rate from all production wells, then, strictly speaking, a steady state flow field, as required by RESSQ, cannot be achieved. However, for large values of time one may assume that quasi-steady flow prevails, thus allowing RESSQ to be used. However, if the sum of the two rates are widely divergent, unexpected and inappropriate results may be found for shorter time periods.

(2) In addition to modeling recharge or injection wells as point sources, RESSQ can model constant head ponds as finite radius sources. This is done by specifying the pond as a recharge well, with radius of the pond specified as the radius of the well. Such sources are however also considered to be fully penetrating.

(3) RESSQ can include a linear no-flow or constant potential boundary using the method of images. A boundary is represented by adding an image well for each real well in the problem, with the boundary located on the perpendicular bisector of the line

connecting each real well/image well pair. For a no-flow boundary the real and image wells have the same flow rate, that is, either both are injection or both are production wells. Since there is no flow through an impervious boundary, the only regional flow allowed in this case is parallel to the boundary. For a constant potential boundary the real well/image well pairs have flow rates equal in magnitude and opposite in sign. In this case the boundary must be an equipotential and the only regional flow allowed is perpendicular to the boundary.

(4) The model requires that the number of injection wells specified must be greater than zero. This is because injection wells act as the starting points for streamlines, so without injection wells no streamline pattern can be drawn. To allow greater flexibility in presenting streamline patterns, zero-flow wells do not affect the velocity field, but provide starting points for streamlines whose paths may help explicate the velocity field created by regional flow and nonzero-flow rate sources and sinks present.

(5) The techniques described in (4) allow the specification of a uniform regional flow by use of a row of zero-flow-rate wells. Streamlines describing regional flow can be drawn by placing a row of zero-flow rate wells perpendicular to the direction of regional flow at a distance relatively far from sources and sinks. The spacing between these wells must be determined as a function of the ratio of source flow rate to regional flow Darcy velocity. A routine (ZQWELL) is incorporated into the model preprocessor to provide for automatic calculation of the required line of zero-flow wells to describe the regional flow. However, the user may find it necessary to experiment with the input for this routine in order to establish a sufficiently small (or sufficiently large) number of such wells to describe the regional flow within the data input limitations of the code.

RESSQ, by neglecting dispersion, provides a sharp-front approximation of contaminant concentration. That is, water injected from a source undergoes no mixing with water already present in the aquifer, but displaces that water without dilution. Output of RESSQ includes plots of the time position of contaminant fronts around sources. Because these represent sharp fronts, the predicted concentration within the fronts is equal to the injection concentration, while the predicted concentration outside the fronts is equal to the ambient aquifer concentration. In actuality, the processes of dispersion and dilution should result in contamination extending beyond the position of the predicted fronts, but with a corresponding dilution of concentration. The user should pay careful attention to this phenomenon in interpreting the results.

If a production well is specified, the time evolution of concentration at the production well will be estimated (provided that at least two stream lines reach the production well during the simulation period). This time evolution is based solely on the number of stream lines from sources captured by the production well, and does not consider the effects of dispersion and dilution.

Input data for RESSQ requires the following information:

NWI: Number of injection wells (> 0), not including zero flow wells automatically specified in routine ZQWELL.

NWP: Number of production wells. May be zero, but see cautions regarding application of the model to non-steady state flow patterns.

C0: Ambient (preexisting) contaminant concentration in the aquifer.

CD: Default concentration of injection wells. This number can be overridden in the specifications for each well (below). However, it is necessary to specify C0 if the user wishes to observe the dimensionless concentration evolution at production wells. In general, the user should specify CD equal to the highest injection well concentration.

UNITC: Units of concentration. This is a character string used to label output. The default value is "Percent."

IZQ: Requests the use routine ZQWELL for automatic calculation of a line of zero flow wells to specify uniform flow (1: yes, 0: no). Generally the user will wish to enter 1 if regional flow is present.

ATTEN: (Default = 1.0). This option is provided for use with surficial sources. In such cases the strength of the contaminant may decrease significantly in the process of percolation through the unsaturated zone. The users may thus specify ATTEN to represent the fraction of the actual source concentration remaining when the flow from the source enters the aquifer.

HEIGHT: Average saturated thickness of aquifer (in feet). This value is assumed to be constant throughout the region of study.

POR: Effective Porosity of the aquifer, expressed as percent ($POR = P \times 100$).

V0: Pore water velocity of uniform flow (ft/day).

ALPHA: Direction of regional flow, in degrees, measured counter-clockwise from the positive X axis.

ADSORB: Adsorption capacity of matrix, equals $(1-1/R)$, where R is the retardation coefficient. The range of ADSORB is 0-1, as $R = V/V_c$, where V is the regional velocity and V_c the apparent velocity of the contaminant.

NFRNTS: Number of contaminant front positions to be calculated for each source (maximum 7).

DATE(1 to NFRNTS): Times at which fronts are to be calculated (in years).

TMAX: Period of study in years. This sets the maximum amount of time for calculating the trace of streamlines, and thus should be substantially greater than the time period of interest. TMAX should be set large enough so that streamlines can be fully drawn throughout the area mapped (e.g., TMAX=200). If you are specifying regional flow through use of zero-flow wells, TMAX should be long enough so that these flow lines can be drawn across the area to be mapped.

DL: The step-length or spatial increment used to trace out the streamlines, in feet. If left blank this defaults to $(XMAX-XMIN)/200$. Using a larger step-length will decrease run time, but will also decrease the resolution of the streamline plot.

NTL: Plot option, set NTL = -1 to suppress plot of streamlines.

NTF: Plot option, set NTF = -1 to suppress plot of pollutant fronts.

XMIN: Origin of area of study, X axis (in feet). It is often convenient, particularly when specifying regional flow, to set up the axes so that $\{X=0, Y=0\}$ is the center of the area of study.

XMAX: Limit of area of study, X axis (in feet).

YMIN: Origin of area of study, Y axis (in feet).

YMAX: Limit of area of study, Y axis (in feet).

The next seven variables control the automatic calculation of a row of zero-flow wells to simulate uniform regional flow. They will be requested only when IZQ=1. The number of ZQWELLS calculated will be displayed after the data is input. If this number is too large you may modify the input and try again. In this case instructions for modification will be displayed.

XREF: X coordinate of arbitrary reference point near the sources and sinks (in feet).

YREF: Y coordinate of the arbitrary reference point.

DIST: Distance from reference point to row of zero flow wells, in feet. Ideally, DIST must be large enough so that near the zero-flow rate wells the streamlines are essentially parallel.

WIDTH: Width of the row of zero-flow wells (in feet). This determines the area that will be covered by the regional flow streamlines.

Q1: Flow rate of the first source (injection well) in gpd. This value will be carried to the source input screen as well.

NSL1: Number of streamlines calculated for the first source.

ITR1: Ratio of NSL1 to the number of streamlines plotted for the first source.

WELLS: The following data must be specified for each source and sink (injection well and source well). The injection wells (sources) must be specified first. Monitor source wells may be specified in order to observe contaminant concentration development.

NAMEW: Name of the well, source or sink (character).

XW: X coordinate of the well (feet).

YW: Y coordinate of the well.

QW: absolute value of flow from/to this well, gpd.

RADDW: radius of well (or pond), in feet. This value will default to 0.2461 ft.

C: concentration of an injecting well in units of UNITC. This will default to C0.

BETA1: angle (degrees) of the first streamline calculated for each injection well. This value can be modified to obtain better streamline definition. The angle is calculated counter-clockwise from the positive X axis.

NSL: number of streamlines calculated for an injection well. Default value is 40. Set NSL = -1 for no streamlines.

ITR: ratio of NSL to number of streamlines actually plotted. Determines the density of the plot. Set ITR = -1 to suppress plotting of streamlines from this well.

INDW: Plot option. Set INDW = -1 to suppress plot of fronts in the case of an injection well, or suppress study of concentration in the case of a production well.

Figures 28 through 29 show input data set examples for RESSQ. Figure 30 illustrates graphical output from this simulation.

RESSQ Input Injection Production

1. Title (Any 80 characters) [A00]	EXAMPLE ONE
2. Number of injection wells (> 0) [I5]	1
3. Number of production wells [I5]	1
4. Ambient concentration in aquifer [E10.4]	0.
5. Default injection concentration [E10.4]	100.
6. Units of concentration (Blank:percent)	
7. System of units [I5]	2
8. Thickness of aquifer (m) [E10.4]	10.
	0 Cancel

Alt-X Exit F4 Help Alt-F3 Close

Figure 26. Input data set 1 for RESSQ

RESSQ Input Injection Production

9. Porosity (percent) [E10.4]	25.
10. Pore water velocity (m/yr) [E10.4]	0.
11. Direction of flow (in degrees) [E10.4]	0.
12. Adsorption capacity(0=no adsorption) [E10.4]	0.
13. Period of study (years) [E10.4]	200.
14. Step length (m) [E10.4]	10.
15. Flag:plot of streamlines [I5]	
16. Flag:plot of fronts [I5]	
	0 Cancel

Alt-X Exit F4 Help Alt-F3 Close

Figure 27. Input data set 2 for RESSQ

RESSQ Input Injection Production

1. Name of production well [A10]

2. x coordinate (m) [E10.4]

3. y coordinate (m) [E10.4]

4. Rate of production (m^3/h) [E10.4]

5. Well radius (Blank: default=7.5 cm)

6. Blank means concentration is to be studied

Alt-X Exit F4 Help Alt-F3 Close

Figure 28. Production well 1 for RESSQ

Utilities Input Data Run PostRESSQ View Files							
model.dat							
EXAMPLE ONE							
1	1	0.	100.	2	0.		
	10.	25.	0.				
Injwell-1	-300.	300.	50.		100.	0.45	3
Prodwell-1	300.	-300.	50.				
3	0.5	2.	4.				
	200.	10.					
	-1000.	1000.	-1000.	1000.			

Alt-X Exit F4 Help Alt <Char> Menu

Figure 29. Viewing the input file

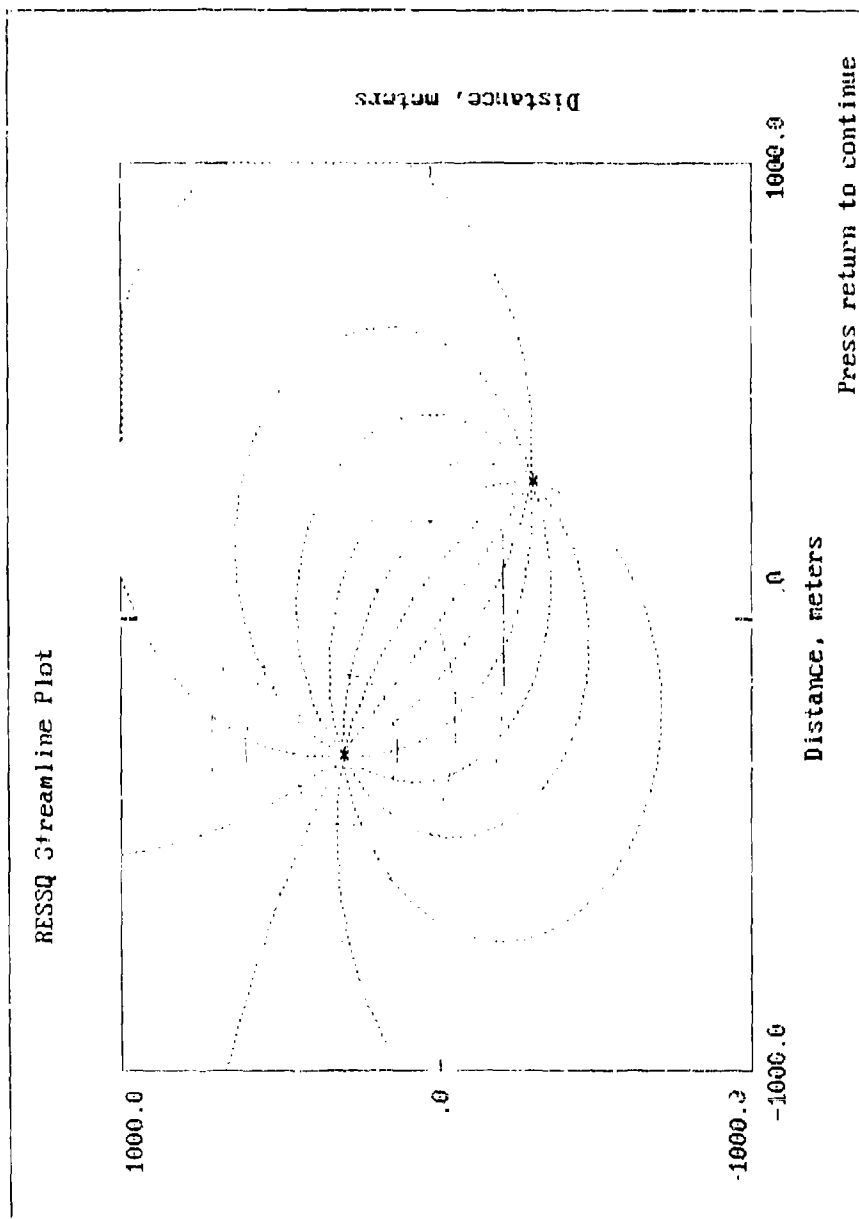


Figure 30. Graphical output from RESSQ

9. USGS MOC

MOC is a two-dimensional model for the simulation of non-conservative solute transport in saturated ground water systems. The model is both general in its applicability and flexible in its design. Thus, it can be applied to a wide range of problems. It computes changes in the spatial concentration distribution over time caused by convective transport, hydrodynamic dispersion, mixing or dilution from recharge, and chemical reactions. The chemical reactions include first order irreversible rate reaction (such as radioactive decay), reversible equilibrium controlled sorption with linear, Freundlich or Langmuir isotherms, and reversible equilibrium controlled ion exchange for monovalent or divalent ions. The model assumes that fluid density variations, viscosity changes, and temperature gradients do not affect the velocity distribution. MOC does allow modeling heterogeneous and/or anisotropic aquifers.

The model couples the ground water flow equation with the non-conservative solute-transport equation. The computer program uses the ADI or SIP procedure to solve the finite difference approximation of the ground water flow equation. The SIP procedure for solving the ground water flow equation is most useful when areal discontinuities in transmissivity exist or when the ADI solution does not converge. MOC uses the method of characteristics to solve the solute transport equation. It uses a particle tracking procedure to represent convective transport and a two-step explicit procedure to solve the finite difference equation that describes the effects of hydrodynamic dispersion, fluid sources and sinks, and divergence of velocity. The explicit procedure is subject to stability criteria, but the program automatically determines and implements the time step limitations necessary to satisfy the stability criteria.

MOC uses a rectangular, block-centered, finite-difference grid for flux and transport calculations. The grid size for flow calculations is limited to 40 rows and 40 columns. The grid size for transport calculations is limited to 20 rows and 20 columns which can be assigned to any area of the flow grid. The program allows spatially varying diffuse recharge or discharge, saturated thickness, transmissivity, boundary conditions, initial heads and initial concentrations and an unlimited number of injection or withdrawal wells. Up to five nodes can be designated as observation points for which a summary table of head and concentration versus time is printed at the end of the calculations.

The program documentation can be found in the following reports:

Konikow, L.F. and J.D. Bredehoeft. 1978. Computer Model of Two-Dimensional Transport and Dispersion in Ground Water. USGS Techniques of Water Resources Investigations, Book 7, Chapter C2.

Goode, D.J. and L.F. Konikow. 1989. Modification of a Method-of-Characteristics Solute Transport Model to Incorporate Decay and Equilibrium-Controlled Sorption or Ion Exchange. USGS Water Resources Investigations Report 89-4030.

MOC has the following **limitations**. The development of the solution required a number of assumptions, and the degree to which field conditions deviate from these assumptions will affect the applicability and reliability of the model. These include the following:

(1) Darcy's law is valid and hydraulic-head gradients are the only significant driving mechanism for fluid flow. Low velocity flow under other conditions is not considered.

(2) Solute transport is dominated by convective transport, an assumption required for the method of characteristics solution of the flow equation.

(3) The porosity and hydraulic conductivity of the aquifer are constant with time, and porosity is uniform in space.

(4) Gradients of fluid density, viscosity, and temperature do not affect the velocity distribution.

(5) No chemical reactions occur that affect the fluid properties or the aquifer properties.

(6) Ionic and molecular diffusion are negligible contributors to the total dispersive flux.

(7) Vertical variations in head and concentration are negligible.

(8) The aquifer is homogeneous and isotropic with respect to the coefficients of longitudinal and transverse dispersivity.

An interactive preprocessor, PREMOC, is included with the program to facilitate user friendly data entry and editing. An example of the graphical output is shown in Figure 31, an enhancement to the original software package..

10. RANDOM WALK

This program provides simulations of a large class of groundwater solute transport problems, including: convection, dispersion, and chemical reactions. The solutions for groundwater flow include a finite difference formulation. The solute transport portion of the code is based on a particle-in-a-cell technique for the convective mechanisms, and a random-walk technique for the dispersion effects.

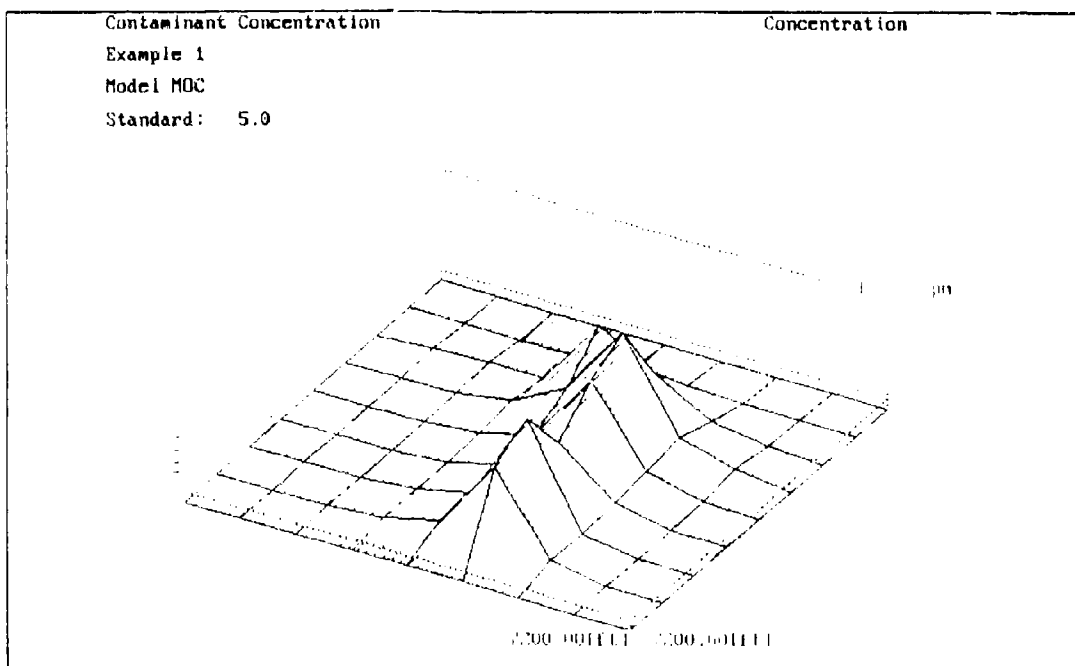


Figure 31. Graphical Output from MOC

The code can simulate one- or two-dimensional nonsteady/steady flow problems in heterogeneous aquifers under water table and/or artesian or leaky artesian conditions. Furthermore, this program covers time-varying pumpage or injection by wells, natural or artificial recharge, the flow relationships of water exchange between surface waters and the groundwater reservoir, the process of groundwater evapotranspiration, possible conversion of storage coefficients from artesian to water table conditions, and flow from springs.

The program also allows specification of chemical constituent concentrations for any segment of the model including, but not limited to, injection of contaminated water by wells, vertically averaged salt-water fronts, leachate from landfill, leakage from overlying source beds of differing quality than the aquifer, and surface water sources such as contaminated lakes and streams. The program documentation can be found in the following report: Prickett, T.A., T.G. Naymik, and C.G. Lonquist, 1981. A "Random-Walk" solute transport model for selected groundwater quality evaluations, Bulletin 65, Illinois State Water Survey, Champaign, Illinois, 103 pages.

Model limitations include:

- (1) As with MOC, concentrations greater than initial conditions are possible, especially when coarse discretizing is used.
- (2) The method may take an unusually large number of particles to produce an acceptable solution for some problems (a maximum of 5000 particles).
- (3) Engineering judgment is an absolute requirement in arriving at an acceptable solution. This is because of the "lumpy" character of the output. Therefore, experience with this technique is needed before one can apply the code successfully to a field situation.

An interactive preprocessor, PREWALK, is included with the program to facilitate user friendly data entry and editing. A screen of the preprocessor is shown in Figure 32.

PREWALK/MAINSCREEN 01

R A N D O M W A L K

ILLINOIS STATE WATER SURVEY - SOLUTE TRANSPORT MODEL

This program can model solute transport in a variety of aquifer conditions: steady or non-steady state, heterogeneous aquifers under watertable and/or artesian or leaky artesian conditions.

The program employs a particle in cell technique to model convective dispersion and a random-walk technique for the dispersion effects. Solutions for groundwater flow are based on finite difference techniques.

Developed by: Thomas A. Prickett
Thomas G. Maynik
Carl G. Loquist

Preprocessor added by: Eric G. Burneson
Department of Civil & Environmental Engineering
Duke University
Durham, North Carolina 27706

Press Return _

Figure 32. A Screen from the RANDOM WALK preprocessor

11. USGS MODFLOW

MODFLOW is a finite-difference model simulating ground water flow in three dimensions, using a block-centered finite-difference approach. Layers can be simulated as confined, unconfined, or a combination of confined and unconfined. Flow from external stresses, such as flow to wells, areal recharge, evapotranspiration, flow to drains, and flow through riverbeds, can also be represented. The finite-difference equations can be solved using either the Strongly Implicit Procedure or Slice-Successive Overrelaxation. The computer program is written in a modular form. It consists of a main program and a series of highly independent subroutines called "modules." The modules are grouped into "packages." Each package deals with a specific feature of the hydrologic system which is to be simulated. This version of MODFLOW includes the following packages:

- BAS1 -- Basic Package
- BCF2 -- Version 2 of Block-Centered Flow Package
- RIV1 -- River Package
- DRN1 -- Drain Package
- WEL1 -- Well Package
- GHB1 -- General Head Boundary Package
- RCH1 -- Recharge Package
- EVT1 -- Evapotranspiration Package
- SIP1 -- Strongly Implicit Procedure Package
- SOR1 -- Slice Successive Over-Relaxation Package
- UTL1 -- Utility Package
- PCG2 -- Version 2 of Preconditioned Conjugate Gradient Package
- STR1 -- Stream Package
- IBS1 -- Interbed-Storage Package
- CHD1 -- Time-Variant Specified-Head Package
- GFD1 -- General Finite Difference Flow Package

The basic model is documented in: McDonald, M.G. and Harbaugh, A.W., 1988, A modular three-dimensional finite-difference ground-water flow model: U.S. Geological Survey Techniques of Water-Resources Investigations Book 6, Chapter A1, 586 pages. The PCG2 Package is documented in: Hill, M.C., 1990, Preconditioned conjugate-gradient 2 (PCG2), a computer program for solving ground-water flow equations: U.S. Geological Survey Water-Resources Investigations Report 90-4048, 43 pages. The STR1 Package is documented in: Prudic, D.E., 1989, Documentation of a computer program to simulate stream-aquifer relations using a modular, finite-difference, ground-water flow model: U.S. Geological Survey Open-File Report 88-729, 113 pages. The IBS1 and CHD1 Packages are documented in: Leake, S.A. and Prudic, D.E., 1988, Documentation of a computer program to simulate aquifer-system compaction using the modular finite-difference ground-water flow model: U.S. Geological Survey Open-File Report 88-482, 80 pages. The GFD1 Package is documented in: Harbaugh, A.W., 1992, A generalized finite-difference formulation for the U.S. Geological Survey modular three-

dimensional finite-difference ground-water flow model: U.S. Geological Survey Open-File Report 91-494, 60 pages. The BCF2 Package is documented in: McDonald, M.G., Harbaugh, A.W., Orr, B.R., and Ackerman, D.J., 1992, A method of converting no-flow cells to variable-head cells for the U.S. Geological Survey modular finite-difference ground-water flow model: U.S. Geological Survey Open-File Report 91-536, 99 pages..

The MAIN program has been modified to include all the packages. The IUNIT assignments for packages not in the original model are:

BCF2 -- IUNIT(1) -- same IUNIT as used for BCF1 because BCF2 replaces BCF1,
PCG2 -- IUNIT(13), GFD1 -- IUNIT(14), STR1 -- IUNIT(18), IBS1 -- IUNIT(19),
CHD1 -- IUNIT(20).

The input unit for the Basic Package is unit 5, which is defined by the assignment of variable INBAS in the MAIN program.

The X array is dimensioned to 350,000. This is large enough for a model having approximately 20,000 cells.

The approximations applied to the flow equation to simulate the effects of a water table (water-table transmissivity calculation, vertical leakage correction, and confined/unconfined storage conversion) were developed using the conceptualization of a layered aquifer system: in which each aquifer is simulated by one model layer and these aquifer layers are separated by distinct confining units. If one attempts to use the water-table transmissivity calculation in the situation where several model layers are simulating the same aquifer and the water table is expected to traverse more than one layer, problems with cells incorrectly converting to no flow may occur. Because the conversion to no flow is irreversible, only declines in the water table can be simulated. Vertical conductance is left constant until a cell converges to no flow, and then is set to zero. This assumes there is a confining layer, which dominates vertical flow, below the model water-table layer. In particular, the model program may have difficulty handling a multilayer simulation of a single aquifer in which a well causes drawdown below the top model layer. The solver may attempt to convert cells to no-flow cells sooner than it should. This could cause the simulation to degenerate.

A shell program is provided for executing the program (Figure 33). The following files are for the example obtained from the original documentation:

twri.5 BAS1 Package input
twri.11 BCF2 Package input
twri.12 WEL1 Package input
twri.13 DRN1 Package input
twri.18 RCH1 Package input
twri.19 SIP1 Package input

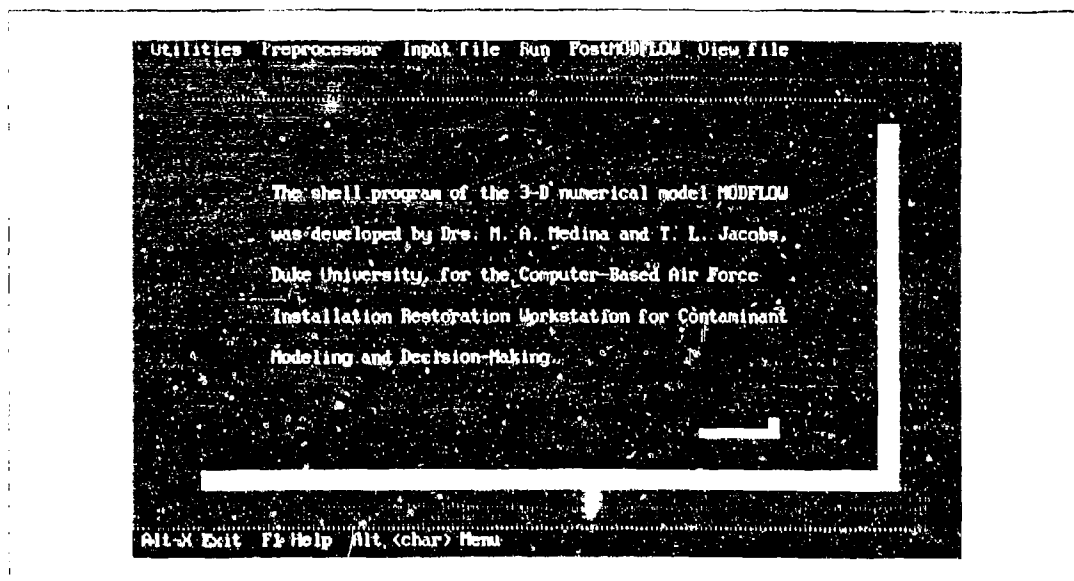


Figure 33. The shell program for MODFLOW

12. SUTRA

SUTRA is written in ANSI-STANDARD FORTRAN-77 and may be compiled and executed under most operating systems and on most computers. Many SUTRA applications require considerable array storage and computational effort. These applications must be carried out on large, fast scalar machines such as mainframes, minicomputers, workstations and 386-or-better microcomputers with math coprocessors and at least a few Mbytes of memory, or on vector/array-processing machines. Applications on 640 Kbyte-limited microcomputer systems are approximately the size of the largest example problem included with this package.

The set of files includes:

- (1) SUTRA main routine (MAIN.FOR);
- (2) 24 SUTRA subroutines contained in three files: (a) USUBS.FOR, with two user-programmable routines, and (b) SUBS1.FOR and SUBS2.FOR with all the other subroutines;
- (3) two mesh data generation routines (MGENREC.FOR and MGENRAD.FOR);
- (4) nine input data sets consisting of three data sets required to run each of three examples from the SUTRA documentation;

- (5) three output data sets with results from these three examples; and
- (6) one routine for calculation of hydrostatic pressure data at specified pressure boundaries (PBCGEN.FOR).

SUTRA is composed of one main routine and 24 subroutines contained in four files listed above, which must first be compiled in FORTRAN-77 and then loaded before running a simulation. Two files must be permanently assigned for the computer installation of the user. Instructions may be found in the main routine, MAIN.FOR. One file captures error output written during file opening. The other file will contain the unit numbers and file names to be assigned as SUTRA input and output files for each simulation. Presently, the error file has unit number 1 and is called SUTRA.ERR, and the simulation units assignment file has unit number 100 and is called SUTRA.FIL. Use of the new simulation units assignment file is described below.

In addition to the two permanently assigned files discussed above, three or four files must be assigned for each simulation in order to run SUTRA. Two are input files and one or two are output files:

UNIT K1: this file contains all of the data necessary for simulation except initial conditions.

UNIT K2: this file contains initial conditions of pressure and concentration or temperature for the simulation.

UNIT K3: the main output of the simulation is placed in this file.

UNIT K4: this file saves simulation results for later restarts. It is needed only if the option to save the final solution for later restart is chosen in UNIT K1 Dataset 4. Data will be written to this file after each ISTORE simulation time steps (NEW feature) in a format equivalent to that required by UNIT K2 so that this file may later be used as UNIT K2 for simulation restart.

These assignments are recorded by the user in the NEW simulation units assignment file which has received a permanent name and unit number in the main program (see above). Presently the file is called SUTRA.FIL and is unit number 1. The required format of this file is:

VARIABLE	FORMAT
Unit Number for K1	(free format)
File Name for K1	(A80)
Unit Number for K2	(free format)
File Name for K2	(A80)
Unit Number for K3	(free format)
File Name for K3	(A80)
Unit Number for K4	(free format)
File Name for K4	(A80)

Three test problems are included in this package. To test the new installation of SUTRA, these problems may be run with the executable file (SUTRA.EXE) included in this package. Results of running the three test problems may then be compared with the three output listings provided in the original documentation package.

SUTRA will provide clear, accurate answers only to well-posed, well-defined, and well-discretized simulation problems. In less-well-defined systems, a SUTRA simulation can help visualize a conceptual model of the flow and transport regime, and can aid in deciding between various conceptual models. SUTRA is not useful for making exact prediction of future responses of the typical hydrogeologic systems which are not well defined. Rather, SUTRA is useful for hypothesis testing and for helping to understand the physics of such a system. On the other hand, developing an understanding of a system based on simulation analysis can help make a set of worthwhile predictions which are predicated on uncertainty of both the physical model design and model parameter values. In particular, transport simulation which relies on large amounts of dispersion must be considered an uncertain basis for prediction, because of the highly idealized description inherent in the SUTRA dispersion process.

Reference materials for the original releases of these codes are:

1- SUTRA - A finite-element simulation model for saturated-unsaturated fluid-density-dependent ground-water flow with energy transport or chemically-reactive single-species solute transport, U.S. Geological Survey Water-Resources Investigations Report 84-4369, 1984, 409pp., by Clifford I. Voss.

2- SUTRA-PLOT - Documentation of a graphical display program for the saturated-unsaturated transport (SUTRA) finite-element simulation model, U.S. Geological Survey Water-Resources Investigations Report 87-4245, 1987, 122pp., by William R. Souza.

13. BIOPLUME II

BIOPLUME II is a two-dimensional model for simulation of transport of dissolved hydrocarbons under the influence of oxygen-limited biodegradation. The code also simulates reaeration and anaerobic biodegradation as a first-order decay in hydrocarbon concentrations. The model is based on the 1987 version of the USGS two-dimensional method of characteristics transport model by Konikow and Bredehoeft. It computes the changes in concentration over time due to convection, dispersion, mixing, and biodegradation. BIOPLUME II solves the transport equation twice: once for hydrocarbon and once for oxygen. As a result, two plumes are computed at every time step. The model assumes an instantaneous reaction between oxygen and hydrocarbon to simulate biodegradation processes. The two plumes are combined using the principle of superposition. The model allows injection wells to be specified as oxygen sources

into a contaminated aquifer. It provides three additional sources of oxygen : initial dissolved oxygen in the uncontaminated aquifer, natural recharge of oxygen across the boundaries, and vertical exchange of oxygen from the unsaturated zone (re-aeration). The model comes with a menu-driven, interactive preprocessor and handles a 20 x 30 cell grid.

Figure 34 shows the preprocessor for BIOPLUME II. Although the model interacts with the user through a series of informative screens, the user is advised to read the user's instructions in the original documentation before running the model. BIOPLUME II is documented in: Rifai et al., "Computer Model of Two-Dimensional Contaminant Transport under the Influence of Oxygen Limited Biodegradation in Ground Water.", User's Manual - Version 1.0. Dept. of Environmental Science and Engineering, Rice University, Houston, Texas, 1987. The model also creates SURFER (Golden Software) compatible output files. The following files are data and output files for one example of model simulation.

Data file: SAMPLE.DAT

Output files: SAMPLE.OUT, HEADS.OUT, OXYGCONC.OUT, and HCCONC.OUT.

Loader
Main Menu

1. Edit file name
2. Edit card 1 (Title)
3. Edit card 2 (Grid/timing parameters)
4. Edit card 3 (Grid/timing parameters)
5. Edit card 4 (Reaction parameters)
6. Edit data set 1 (Observation wells)
7. Edit data set 2 (Pump/Inject wells)
8. Edit data set 3 (Transmissivity map)
9. Edit data set 4 (Thickness map)
10. Edit data set 5 (Recharge map)
11. Edit data set 6 (Nodeid map)
12. Edit data set 7 (Nodeid code definitions)
13. Edit data set 8 (Water table elevations)
14. Edit data set 9 (Initial hydrocarbon conc.)
15. Edit data set 10 (Initial oxygen conc.)
16. Edit data set 11 (Pumping periods)
17. Write data to file
18. Quit

Enter the number of your choice (1..18) ...

Figure 34. Preprocessor for BIOPLUME II

14. ODAST IN MONTE CARLO MODE

The program ODAST evaluates the one dimensional analytical solute transport solution considering convection, dispersion, decay and adsorption in porous media (Javandel et al., 1984). The program has been modified to facilitate Monte Carlo analysis. In Monte Carlo mode, the input concentration and regional flow velocity both become random variables, and the cumulative frequency estimated over these and other random parameters should provide a reasonable estimate of the average risk. An example is provided in section III(G).

The preprocessor developed for ODAST in Monte Carlo mode follows a standard format that is used for most of the models in the system. This consists of presentation of a number of screens, with input slots to be filled. The data to be input for ODAST in Monte Carlo mode are as shown in the following screens.

ODASt Input

1. Number of x positions [15]

Values of distance x from the source(m)[D10.4]:

2. 1st : <input type="text" value="500.1"/>	3. 2nd : <input type="text"/>	4. 3rd : <input type="text"/>
5. 4th : <input type="text"/>	6. 5th : <input type="text"/>	7. 6th : <input type="text"/>
8. 7th : <input type="text"/>	9. 8th : <input type="text"/>	10. 9th : <input type="text"/>
11. 10th : <input type="text"/>	12. 11th : <input type="text"/>	13. 12th : <input type="text"/>
14. 13th : <input type="text"/>	15. 14th : <input type="text"/>	16. 15th : <input type="text"/>
17. 16th : <input type="text"/>	18. 17th : <input type="text"/>	19. 18th : <input type="text"/>

Alt-X Exit F4 Help Alt-F3 Close

Figure 35. Input data set 1 for ODASTMC

ODAST Input

1. Number of time points [15]

Values of time to calculate C/C0(years)[D10.41]:

2. 1st : <input type="text" value="10"/>	3. 2nd : <input type="text" value=""/>	4. 3rd : <input type="text" value=""/>
5. 4th : <input type="text" value=""/>	6. 5th : <input type="text" value=""/>	7. 6th : <input type="text" value=""/>
8. 7th : <input type="text" value=""/>	9. 8th : <input type="text" value=""/>	10. 9th : <input type="text" value=""/>
11. 10th : <input type="text" value=""/>	12. 11th : <input type="text" value=""/>	13. 12th : <input type="text" value=""/>
14. 13th : <input type="text" value=""/>	15. 14th : <input type="text" value=""/>	16. 15th : <input type="text" value=""/>
17. 16th : <input type="text" value=""/>	18. 17th : <input type="text" value=""/>	19. 18th : <input type="text" value=""/>

Alt-X Exit F4 Help Alt-F3 Close

Figure 36. Input data set 2 for ODASTMC

ODAST Input

Input mean value (MU), standard deviation, (SD) and parameter distribution type (PDT)

	MU	SD	PDT
1. Time of waste recharge(years)[D10.41]:	<input type="text" value="10"/>	<input type="text" value="0"/>	<input type="text" value="2"/>
2. Pore water velocity (m/d) [D10.41]:	<input type="text" value="0.064"/>	<input type="text" value="0.0864"/>	<input type="text" value="2"/>
3. Longitudinal dispersivity (n)[D10.41]:	<input type="text" value="1.75"/>	<input type="text" value="0.175"/>	<input type="text" value="2"/>
4. Diffusion coefficient (m ² /d)[D10.41]:	<input type="text" value="6.1E-5"/>	<input type="text" value="6.1E-6"/>	<input type="text" value="2"/>
5. Source concentration [D10.41]:	<input type="text" value="1"/>	<input type="text" value="0"/>	<input type="text" value="2"/>

Alt-X Exit F4 Help Alt-F3 Close

Figure 37. Input data set 3 for ODASTMC

ODAST Input

Input mean value (MU), standard deviation, (SD) and parameter distribution type (PDT)

	MU	SD	PDT
1.Bulk mass density (g/cm ³) [D10.4]:	1.367	0.1367	2
2.Porosity [D10.4]:	0.5	0.05	2
3.Distribution coeff. (cm ³ /g)[D10.4]:	2.29	0.229	2
4.Radioactive decay factor [D10.4]:	0.	0.	2
5.Decay factor of the source [D10.4]:	0.	0.	2

OK Cancel

Alt-X Exit F4 Help Alt-F3 Close

Figure 38. Input data set 4 for ODASTMC

ODAST Input

1.Target concentration to evaluate [D10.4]	0.05
2.Number of Monte Carlo runs [I5]	1000
3.Observation point of X [I5]	1
4.Observation point of I [I5]	1
5.Name of contaminant [A10]	TCE
6.Name of site [A10]	TEST

OK Cancel

Alt-X Exit F4 Help Alt-F3 Close

Figure 39. Input data set 5 for ODASTMC

15. TDAST IN MONTE CARLO MODE

The model TDAST evaluates the two-dimensional analytical solute transport solution, considering convection, dispersion, decay and adsorption in porous media (Javandel et al., 1985). The program has been modified to facilitate Monte Carlo analysis. TDAST in Monte Carlo mode has a similar preprocessor to that of TDAST. The data input is thus essentially the same as that for TDAST, with some modifications, as shown in the following screens.

TDAST Input

1. Distance x from the source (m) [F10.4]:	500.
2. Distance y from the source (m) [F10.4]:	250.
3. Time t elapsed since the beginning (day) [F10.4]:	3650.
4. Number of Monte Carlo Runs [I5]:	50
5. Seed for random number generator [I5]:	100
6. Maximum allowable concentration [F10.4]:	1.

0 Cancel

Alt-X Exit F4 Help Alt-F3 Close

Figure 40. Input data set 1 for TDASTMC

TDAST Input

Input mean value (MU), standard deviation, (SD) and parameter distribution type (PDT)

	MU	SD	PDT
1. Pore water velocity (m/day) (F10.4):	0.1	0.01	2
2. Longitudinal dispersivity(m)(F10.4):	50.	5.	2
3. Transverse dispersivity(m)(F10.4):	5.	0.	2
4. Diffusion coefficient(m ² /d)(F10.4):	0.	0.	2
5. Source concentration (F10.4):	5000.	0.	2
5. Half length of source (m) (F10.4):	50.	0.	2

0 Cancel

Alt-X Exit F4 Help Alt-F3 Close

Figure 41. Input data set 2 for TDASTMC

TDAST Input

Input mean value (MU), standard deviation, (SD) and parameter distribution type (PDT)

	MU	SD	PDT
1. Bulk mass density (g/cm ³) (F10.4):	2.5	0.	2
2. Porosity (F10.4):	0.3	0.	2
3. Distribution coeff. (cm ³ /g)(F10.4):	0.	0.	2
4. Radioactive decay factor (F10.4):	0.	0.	2
5. Decay factor of the source (F10.4):	0.	0.	2

0 Cancel

Alt-X Exit F4 Help Alt-F3 Close

Figure 42. Input data set 3 for TDASTMC

16. MOC IN MONTE CARLO MODE

MOC in Monte Carlo accounts for the most important only some of the many possible sources of uncertainty are considered in this procedure. These were selected on the basis of a sensitivity analysis, under the assumption that the hydraulic heads along the boundaries are exactly known. Thus the Monte Carlo method is designed to be most applicable for the specific case of analysis of proposed hazardous waste sites. Of particular interest in this method is the specification of a spatially covariant hydraulic conductivity random field, which is well adapted to the simulation of the natural uncertainty in this parameter, where it is expected that hydraulic conductivity values will tend to show a higher degree of similarity between nodes that are closer together in space. The Monte Carlo procedure also conceives of a situation during which contaminant input begins following the failure of a containment structure, prior to which there is essentially no input from the source. This conception is most applicable to the analysis of a proposed hazardous waste landfill, in which the analyst must consider the possibility of contamination resulting from failure of the landfill liner, thus the following elements of uncertainty are included:

(1) Site Reliability Model

Given that the probability that the landfill will fail in any year is p , then t_f , the year in which the landfill liner fails is geometrically distributed with parameter p :

$$Prob(t_f/p) = p(1-p)^{t_f-1} \quad (5)$$

It is very likely that the value of p can be estimated only with limited precision. To reflect this uncertainty, we assume that the parameter p is a priori beta distributed with parameters a and b :

$$p \sim Beta(a,b) \quad (6)$$

(2) Leachate Release Concentration

Given that a failure has occurred, the probability of the amount/ characteristics of the released point source contaminant, C_L , at time t_f is a priori normally distributed with mean u_c and variance v_c :

$$(C_L/t_f) \sim N(u_c, v_c) \quad (7)$$

As in most numerical models, areal sources will be assumed to be represented by a number of point sources.

(3) Hydraulic Conductivity Random Field

It is well documented that the spatial variability of hydraulic conductivity can have a significant effect on the field-length dispersion of contaminant plumes and that hydraulic conductivity is lognormally distributed (Freeze, 1975; Smith and Schwartz, 1980, 1981). We assume a two level stochastic model to reflect both natural and parameter uncertainty in the hydraulic conductivity field distribution. For the case of m nodes, it is assumed that $\underline{K} = \ln(K_0)$, the $(m \times 1)$ vector of the natural logarithm of the hydraulic conductivity, follows an m -dimension normal multivariate distribution with mean $u_k \underline{b}$ and covariance $v_k B$:

$$\underline{K} \sim N(u_k \underline{b}, v_k B) \quad (8)$$

where $\underline{b} = (1, 1, \dots, 1)^T$, is an $m \times 1$ vector of ones, B is an $m \times m$ matrix whose diagonal elements are equal to one, and whose ij -th off-diagonal elements are given by the expression $\exp(-d_{ij}/d_0)$, where d_{ij} is the distance between the i th and j th point and d_0 is the correlation length. In addition, in order to reflect uncertainty about the parameters of the distribution, it is assumed that a priori u_k conditioned on v_k is normally distributed with mean M and variance v_k / τ :

$$(u_k / v_k) \sim N(M, v_k / \tau) \quad (9)$$

and $(1/v_k)$ is gamma distributed with parameters c and d ,

$$(1/v_k) \sim \text{Gamma}(c, d) \quad (10)$$

In practice, v_k is generated from $C0/(2X)$, where X is an inverse chi-square deviate.

(4) Background Concentration

The pre-existing concentration of solute in the aquifer, prior to landfill failure, C_B , is assumed to be uniform throughout the aquifer and specified by a log-normal distribution:

$$\ln(C_B) \sim N(u_B, v_B) \quad (11)$$

Note that this requires that the background concentration cannot be exactly zero.

The model allows the specification of a time-varying pumping schedule through the specification of a number of pumping periods. During each of these periods the

pumping occurs at a constant rate. However, differing pumping configurations may be specified for subsequent pumping periods. For Monte Carlo simulation the model should be run in steady-state mode with only one pumping period specified.

The input data is organized by card images, as follows:

- card 1. Title
- card 1a. Monte Carlo card I
- card 1b. Monte Carlo card II. . . .
- card 2. Control card I.
- card 2a. Control card Ia (optional)
- card 3. Control card II
- card 3a. Control card IIa (optional)
- data set 1. Observation points.
- data set 2. Wells
- data set 3. Transmissivity.
- data set 4. Aquifer thickness
- data set 5. Recharge/discharge.
- data set 6. Node identification matrix.
- data set 7. Instruction for node id's .
- data set 8. Initial head.
- data set 9. Initial concentration . . .
- data set 10. Additional pumping periods.

The two Monte Carlo control cards are required when the model is used in Monte Carlo mode. When the preprocessor for MOC is accessed and the site has not been previously analyzed using this model, a default data set may be loaded to guide data input. If previous analysis has occurred the previously formulated data set will be reloaded.

Details for the input "cards" follow:

CARD 1. TITLE

TITLE: Title of the problem and contaminant studied (to 80 characters).

CARD 1A. MONTE CARLO CARD 1. Required only for Monte Carlo applications.

JTER: Number of Monte Carlo iterations to run. Ideally, JTER should be set to a relatively large number in order to yield good definition of the cumulative frequency histogram. However, MOC is quite slow when run in Monte Carlo mode on a PC. The user is advised to initially test the input data by running the model with JTER set to a small number. A complete run can later be undertaken at a time when the computer can be left to run overnight.

BACKM: Mean of the log background concentration of solute. As presently formulated, MOC in the Monte Carlo mode requires the specification of a non-zero background concentration. If there is not known to be any background concentration present this value may be set to the detection limit of the solute species.

SBACK: Standard deviation of BACKM. The background concentration throughout the grid is modeled as a log-normal process.

CARD 1b. Monte-Carlo data card II. Required for Monte Carlo applications.

TARGY: Time horizon for simulations (years). This is the total time of simulation. Failure of the landfill liner may or may not occur within this time horizon.

UALPHA: MOC in the Monte Carlo mode presumes that contamination may commence at an unknown date within the scope of the simulation, as with the failure of the landfill liner. The probability of failure in a given year is described by a geometric distribution with parameter p , while p follows a Beta distribution. UALPHA describes the lower bound (a) of this distribution.

UBETA: Upper parameter (b) of the Beta distribution. To simulate a fixed time of failure, set TARGY to cover the time from known failure to the time of interest, and set UALPHA and UBETA to 1.

RELCM: Mean release concentration of solute (u_c), given failure, modeled as a normal process.

SRELC: Standard deviation of RELCM ($\sqrt{V_c}$).

The next five variables relate to the generation of the spatially covarying hydraulic conductivity field, which has covariance $v_k B$. The variable v_k is generated as $C0/(2X)$, where X is an inverse chi-square deviate, where the conditional mean, u_k , is generated by a normal process with variance v_k / τ .

NOBS: Degrees of freedom for the inverse chi-square deviate. This may be interpreted as the equivalent number of observations for a prior distribution on the hydraulic conductivities.

KPRM: Transmissivity is modeled as a log-normal process, with spatial covariance throughout the grid. KPRM is the mean log transmissivity (M).

CO: May be interpreted as the sum of squares for the transmissivity prior.

TAU: Divisor (τ), relating the variance of the mean hydraulic conductivity to the covariance of the hydraulic conductivity field. As stated above, $\underline{K} \sim N_m(u_k \underline{b}, v_k B)$, and $u_k/v_k \sim N(M, v_k/\tau)$.

DL: Integral scale (d_0): the correlation length (in feet) for the hydraulic conductivity covariance matrix B, the off-diagonal elements of which are given by $\exp(-d_x/d_0)$. For information on this parameter the user may refer to Hoeksema and Kitanidis (1985).

CARD 2. CONTROL CARD 1.

NTIM: Maximum number of time steps in a pumping period (limit 100).

NPMP: Number of pumping periods to be specified.

NX: Grid set-up, number of nodes in x-direction.

NY: Number of nodes in y-direction.

NPMAX: Maximum number of particles traced (limit 6400).

NPNT: Number of time steps between printouts. In the Monte Carlo mode a printout will be made after the first run. Subsequent printouts can be suppressed by specifying $NPNT > NTIM$.

NITP: Number of iteration parameters (usually between 4 and 7).

NUMOBS: Number of observation points to be specified in a following data set (maximum 5).

ITMAX: Maximum number of iterations to be used in the ADI (alternating direction implicit) solution procedure of the flow equation (usually between 100 & 200). A warning will be issued if this value is exceeded without convergence. The authors note that it may be difficult to obtain a solution using the iterative ADI procedure for cases of steady-state flow when internal nodes of the grid have zero transmissivity and for cases in which the transmissivity is highly anisotropic.

N^o EC: Number of pumping or injection wells to be specified. One such well is allowed per node.

NPTPND: Initial number of particles per node (allowable values 1,4,5,8,9, or 16). Increasing NPTPND decreases the mass balance error, but also substantially increases required CPU time for execution. The user can examine reported mass balance errors on the output. There will often be a trade-off between NPTPND and CELDIS in determining the accuracy, stability and time requirements of the solution, depending on whether or not CELDIS is the limiting stability criterion. The authors recommend specifying NPTPND as 4 or 5 for initial model calibration, then increasing NPTPND to 9 or 16 for final runs when maximum accuracy is desired. Higher values of NPTPND may not however be practical in Monte Carlo mode, due to length of execution time required.

NCODES: Number of node identification codes (maximum 10). These codes will be used to specify characteristics of identified nodes in a later data set.

NPNTMV: Particle movement interval (IMOV) for printing chemical data (in Monte

Carlo mode enter 0 to suppress printing after the first Monte Carlo run; 99 to print at the end of each run).

NPNTVL: Option for printing computed velocities (0: do not print, 1: print for first time step, 2: print for all time steps).

NPNTD: Option for printing computed dispersion coefficients (0, 1 or 2 - same as for NPNTVL).

NPDELC: Should changes in concentration be printed (1:yes, 0:no).

NPCHV: Option to write velocity data on unit 7 (0, 1 or 2).

NREACT: Should Retardation and Radioactive Decay be included?

CARD 2a. CONTROL CARD Ia (optional). This card allows the specification of a subgrid so that solute transport may be specified on a smaller grid than calculation of flow.

MX: X coordinate, within the primary grid, of the UPPER-LEFT node of the transport subgrid.

MY: Y coordinate, within the primary grid, of the UPPER-LEFT node of the transport subgrid.

MMX: X coordinate of LOWER-RIGHT node of transport subgrid.

MMY: Y coordinate of LOWER-RIGHT node of transport subgrid.

CARD 3. CONTROL CARD II.

PINT: Pumping period, in years. If more than one pumping period is specified data will be later requested for the subsequent periods.

TOL: Convergence criteria for the ADI iterative solution procedure (usually within 0.01).

POROS: Effective porosity of the medium, assumed constant throughout the aquifer.

BETA: Characteristic length (longitudinal dispersivity) in feet.

S: Storage coefficient (set 0 for steady flow problems).

TIMX: Time increment multiplier for transient flow problems. Ignored if S=0.

TINIT: Size of the initial time in seconds. This is required only for transient flow problems, and is ignored if S=0.

XDEL: Width of finite-difference cell in x-direction, in feet.

YDEL: Width of finite-difference cell in y-direction, in feet.
DLTRAT: Ratio of transverse to longitudinal dispersivity.

CELDIS: Maximum cell distance per particle move (between 0 and 1). Increasing CELDIS generally decreases CPU requirements. Effects on mass balance will be problem-dependent, but will not affect the solution in problems for which CELDIS is not the limiting stability criterion. Further, if CELDIS is reduced to too small a level oscillations may be found in the initial time period of the solution, particularly if the initial distance that a particle can move is less than the spacing between particles (determined by NPTPND). The authors recommend setting CELDIS to 0.75 or 1.0 for initial calibration, then changing CELDIS to 0.50 for final runs.

ANFCTR: Anisotropy factor, ratio of T_{yy} to T_{xx} .

CARD 3a. CONTROL CARD 11a (optional). Required only when decay or adsorption are included.

DK: distribution coefficient of the solute.
RHOB: bulk density of the solid.
THALF: half-life of the solute (in seconds).

DATA SET 1. OBSERVATION POINTS. This data set specifies the location of observation wells at which detailed output will be provided. In Monte Carlo applications these will be the points at which cumulative concentration frequencies are calculated. For each observation point the user must enter:

IXOBS: grid index in x of the observation point.
IYOBS: grid index in y of the observation point.

DATA SET 2. WELLS. Specifies pumping and injection wells. For each well, the user must enter:

IX: grid index in x of the well.
IY: grid index in y of the well.
REC: pumping (>0) or injection (<0) rate of the well, in ft^3/sec .
CNRECH: solute concentration of injected water. Required only for injection wells.

DATA SET 3. TRANSMISSIVITY (deterministic mode only).

DATA SET 4. AQUIFER THICKNESS.

DATA SET 5. RECHARGE/DISCHARGE.

DATA SET 6. NODE IDENTIFICATION MATRIX.

DATA SET 8. INITIAL HEADS.

DATA SET 9. INITIAL CONCENTRATION (deterministic mode only).

For each of these data sets the user will first be queried for the following:

INPUT: The parameter is (0: constant, 1: varies in space).

FCTR: Constant value (or multiplication factor) for the parameter. If INPUT=1 the user will then be queried for values throughout the grid. Note that the preprocessor allows block assignment of values to areas on the grid. This procedure is described in the on-screen Help available from the preprocessor.

DATA SET 7. INSTRUCTION FOR NODE ID'S. The NODE ID's identify special input for the appropriately coded nodes. For each of the codes the user is queried for the following:

ICODE: code number for this node ID. Code 2 cannot be used here, as this is reserved for generated releases in Monte Carlo applications.

FCTR1: leakance at the coded node.

FCTR2: concentration at the coded node.

FCTR3: recharge at the coded node.

OVERRD: Set OVERRD=0 to preserve values of RECH specified in Data Set 5.

DATA SET 10. ADDITIONAL PUMPING PERIODS. If more than one pumping period is specified, the following data must be entered for each additional pumping period. (See above, Card 2, for more detailed discussion of these variables).

ICLK: Should data be revised for this period(1:yes, 0:no).

NTIM: Maximum number of time steps in the pumping period (limit 100).

NPNT: Number of time steps between printouts.

NITP: Number of iteration parameters (usually between 4 & 7).

ITMAX: Number of iterations in ADIP (usually between 100 and 200).

NREC: Number of pumping or injection wells to be specified.

NPNTMV: Particle movement interval (IMOV) for printing chemical data (enter 0 for printing at the end of the simulation).

NPNTVL: Option for printing computed velocities(0: do not print, 1: print for first time step, 2: print for all time steps).

NPNTD: Option for printing computed dispersion coefficients (0, 1 or 2 - same as above).

NPDELC: Should changes in concentration be printed? (1:yes, 0:no).

NPNCHV: Option to write velocity data on unit 7(0,1 or 2).

PINT: Length of pumping period in years.

TIMX: Time increment multiplier for transient flow problems.

TINIT: Size of initial time in seconds for transient flow problems.

17. REMEDIATION OPTIMIZATION

The program OPTIM provides an optimization design for a pump-and-treat remediation scheme, including the optimal well locations, pumping rates, and cost analysis. First of all, the main program extracts aquifer flow and contaminant characteristics from files created by running MOC. The user is asked to enter the minimum acceptable contaminant concentration in order that a contaminant plume may

be defined. In addition, the user enters the location of an observation well and a time frame for the remediation effort. Due to the limitations of DOS, the full remediation optimization (with excellent graphics windows) has been developed for the UNIX version.

The observation well may be a domestic well or other point of contaminant level concern. The user may choose to locate the pumping well(s) manually or automatically. The user may choose any number of different remediation schemes to be considered and, if the manual location option is chosen, the number of wells in each scheme. If the user chooses to have the wells automatically located, a choice is made between an areal or a hydraulic barrier remediation approach. Following the location of the wells, the pumping rates are assigned, either manually or automatically, to each well. The cost of each remediation scheme is calculated. Finally, for each remediation scheme, the location of the wells, pumping rates, radii of influence, and cost are printed.

This program gives the following information concerning remediation strategy:

(1) Well locations

There are two options: areal remediation scheme and hydraulic barrier remediation scheme. If the areal remediation scheme is chosen, the X coordinates of the wells are assigned by the following equation:

$$X(j) = \text{Min}X + \frac{\text{Dim}X}{2i} (2j-1) \quad (12)$$

where X represents the x coordinate of well j, i is the number of wells in the remediation scheme, MinX is the minimum x coordinate of the contaminant plume, and DimX is the maximum dimension of the plume in the x direction. The above equation locates the wells equidistant over the length of the plume in the x direction. The Y coordinates of the wells are assigned by finding the dimension of the plume in the y direction at X(j). The well is then located in the center of the y plume dimension at the x coordinate of the well.

If the hydraulic barrier remediation scheme is chosen, the wells are located in a line such that they create a hydraulic wall toward which the contaminants flow. The wells extend perpendicular to the primary direction of flow between the contaminant plume minimum and maximum points in the direction parallel to flow. The equations for locating wells given flow in the +x direction are as follows:

$$X(j) = \text{Max}X - \frac{\text{Dim}Y}{2i} \quad (13)$$

$$Y(j) = \text{Min}Y + \frac{\text{Dim}Y}{2i} (2j - 1) \quad (14)$$

where MaxX is the maximum x coordinate of the contaminant plume and DimY is the maximum dimension of the plume in the y direction.

(2) Pumping rates

Pumping rates are chosen manually by the user or calculated automatically by the program for each well based on a radius of influence. For automatic calculation of pumping rates, the desired radius of influence was assumed to be one-half of the distance to the closest well. The MOC model makes the following assumption based on storage coefficient, S, whether an aquifer is confined or unconfined:

if $S < 0.005$ then assume $\partial b / \partial t = 0 \Rightarrow$ confined aquifer

if $S \geq 0.005$ then assume $\partial b / \partial t = \partial h / \partial t \Rightarrow$ unconfined aquifer

The equilibrium pumping rate equation for a confined aquifer (DeMarsily, 1986) is also used:

$$Q = 2\pi T \frac{(H - h)}{\ln(R/r)} \quad (15)$$

where T is the transmissivity, H is the hydraulic head prior to pumping, h is the hydraulic head in the vicinity of the well borehole, R is the radius of influence of the well, and r is the radius of the borehole. The equilibrium equation for an unconfined aquifer is calculated as:

$$Q = \pi K \frac{(H^2 - h^2)}{\ln(R/r)} \quad (16)$$

where K is the hydraulic conductivity ($T = Kb$). Sixty-seven percent drawdown is the maximum economical well operation since approximately 90 percent of a well's yield is achieved at sixty-seven percent drawdown (Driscoll, 1986). However, the drawdown may vary with the radius of influence. An approximate way of calculating pumping rates without knowing the drawdown and influence radius is through the desired darcy velocity along the boundary of influence radius:

$$Q = 2\pi R b v$$

(17)

Pumping rates and radii of influence are calculated based on a drawdown of fifty percent.

(3) Cost analysis

The cost of drilling is estimated to be \$20 per vertical linear foot (Waier, 1992). The cost of pumps is related to the horsepower of the pump. For each well, the horsepower of the pump is calculated based on the total dynamic head, pump efficiency, and the pumping rate (Driscoll, 1986). The total dynamic head is assumed as the depth from the surface to the center of the saturated thickness of the aquifer. The pump efficiency is assumed to be 65 percent.

Since the program is based on Thiem (equilibrium) equation, it can not be applied except within reasonable distances of a well: steady radial flow to a well is only achieved near the well where the hydraulic conductivities are homogeneous. Therefore, it is less accurate when applied to a case where a large amount of contaminant exists and a very high pump rate is needed. The user should consider this program as a tool for visualizing the possible remediation schemes rather than obtaining some precise features of the pump-and-treat system.

G. EXAMPLE APPLICATIONS

In this section we provide several examples of the use of the system in contaminant transport modeling, adapted from field-site studies.

1. Example One: ODAST

The one-dimensional analytical model ODAST was prepared to illustrate the relationship between OU 3 (Operable Unit 3, Hill Air Force Base, Utah) sources and contaminant migration. The model assumes that the aquifer is homogeneous and isotropic with steady-state uniform groundwater flow at constant velocity. It calculates the contaminant concentration at any time, at any distance from the source based on the length of time the contaminant was injected into groundwater, and it adjusts the concentration for dispersion and retardation. Table 3 list input data requirements.

Table 3. Input Data Summary, ODAST Hill AFB Example

Data 1:	Input	Explanation
1. Number of x positions	18	Assume source of TCE located at monitoring well ESE-9. The 18 x positions are southwest from the source.
2. 1st value of distance (x) from the source	30.5	30.5 meters=100 feet
3. 2nd value of x	61.0	61.0 meters=200 feet
4. 3rd value of x	91.4	91.4 meters=300 feet
5. 4th value of x	121.9	121.9 meters=400 feet
6. 5th value of x	152.4	152.4 meters=500 feet
7. 6th value of x	182.9	182.9 meters=600 feet
8. 7th value of x	213.4	213.4 meters=700 feet
9. 8th value of x	243.8	243.8 meters=800 feet
10. 9th value of x	274.3	274.3 meters=900 feet
11. 10th value of x	304.8	304.8 meters=1000 feet
12. 11th value of x	457.2	457.2 meters=1500 feet
13. 12th value of x	609.6	609.6 meters=2000 feet
14. 13th value of x	762.2	762.2 meters=2500 feet
15. 14th value of x	914.6	914.6 meters=3000 feet
16. 15th value of x	1067.1	1067.1 meters=3500 feet

17. 16th value of x	1219.5	1219.5 meters=4000 feet
18. 17th value of x	1372.0	1372.0 meters=4500 feet
19. 18th value of x	1524.4	1524.4 meters=5000 feet
Data 2:		
1. Number of time points	1	Sources released from 1940
2. 1st value of time at which concentration is required	51.	The elapsed time is 51 years. The time at which concentration is evaluated is 1991.
Data 3:		
1. Longitudinal dispersion coefficient	5.09	(1) Dispersion coefficient=velocity x dispersivity (2) Dispersivity=200 feet(for alluvial sediments) (3) Dispersion coefficient= 20000 ft**2/yr= 5.09 m**2/day
2. Pore water velocity	0.0835	(1) Groundwater velocity= 100 ft/yr= 0.0835 m/day (2) From slug test results, most of the velocities were less than 100 ft/yr.
3. Retardation factor	4.5	The minimum retardation factor for TCE is 4.5 (estimated from the percent of organic carbon in the soil)
4. Total period of waste recharge	36.	A source released contaminants to the ground-water for 36 years (1940 to 1976)
5. Radioactive decay factor	0.	
6. Decay factor of the source	0.	

The input file for ODAST: MODEL.DAT is

```

18  1
   30.5  61.0  91.4  121.9  152.4  182.9
   213.4  243.8  274.3  304.8  457.2  609.6
   762.2  914.6  1067.1  1219.5  1372.0  1524.4
   51.
   5.09  0.0835  4.5  36.  0.  0.
0

```

The output file for ODAST: MODEL.OUT is

SOURCE CONCENTRATION C0 = 1.00

CONCENTRATION (C) FOR
V = 08 D = 5.09 R = 4.5 LAMBDA = .000 ALPHA = .000 T0 = 36.0

T(YEARS) X = 31 X = 61 X = 91 X = 122 X = 152 X = 183

51.0 2373D+00 3286D+00 4191D+00 5002D+00 5637D+00 6044D+00

CONCENTRATION (C) FOR
V = 08 D = 5.09 R = 4.5 LAMBDA = .000 ALPHA = .000 T0 = 36.0

T(YEARS) X = 213 X = 244 X = 274 X = 305 X = 457 X = 610

51.0 6205D+00 6135D+00 5870D+00 5459D+00 2738D+00 8733D-01

CONCENTRATION (C) FOR
V = 08 D = 5.09 R = 4.5 LAMBDA = .000 ALPHA = .000 T0 = 36.0

T(YEARS) X = 762 X = 915 X = 1067 X = 1220 X = 1372 X = 1524

51.0 1745D-01 2140D-02 1578D-03 6844D-05 1803D-06 2761D-08

Elapsed time 6000E-01 seconds

The concentration profile (breakthrough curve) is presented in Figure 45.

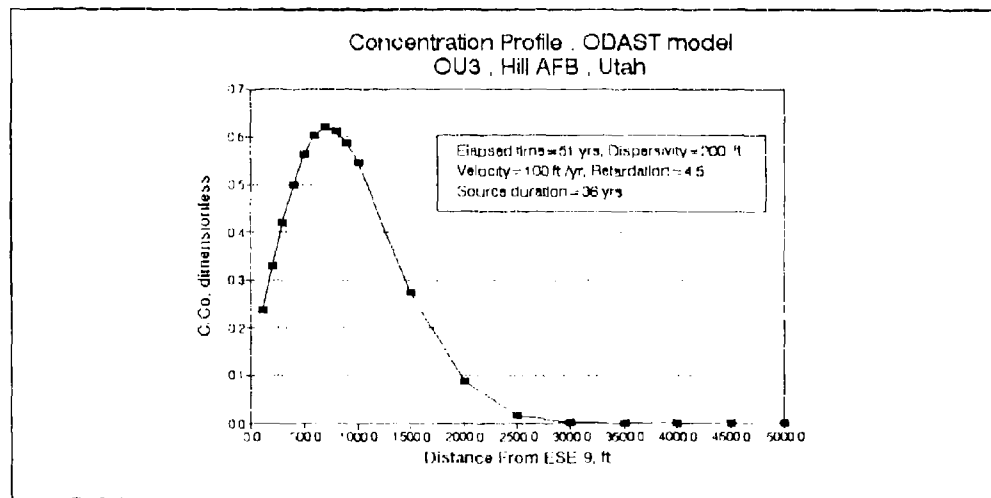


Figure 45. Application of ODAST to OU3 Hill AFB

2. Example Two: RESSQ

RESSQ was used to simulate two-dimensional advective transport under the injection, extraction, and natural-gradient condition of the tracer experiments. The field site is in the Moffett Naval Air Station, Mountain View, California (Roberts, et al., 1990). The RESSQ model was used to estimate (1) the areal extent of the injection fluid front that develops around the injection well and observation wells, (2) the fluid residence times from the injection well to the observation wells, and (3) the degree of recovery of the injected fluid at the extraction well. A sketch of the well fields is presented in Figure 46, for fluid injection at a rate of 0.5 liter/min at three wells, extraction rate of 8 liters/min, regional groundwater flow of 300 m/yr, a porosity of 0.35, and an aquifer thickness of 1.2 meters. Table 4 summarizes the input data requirements.

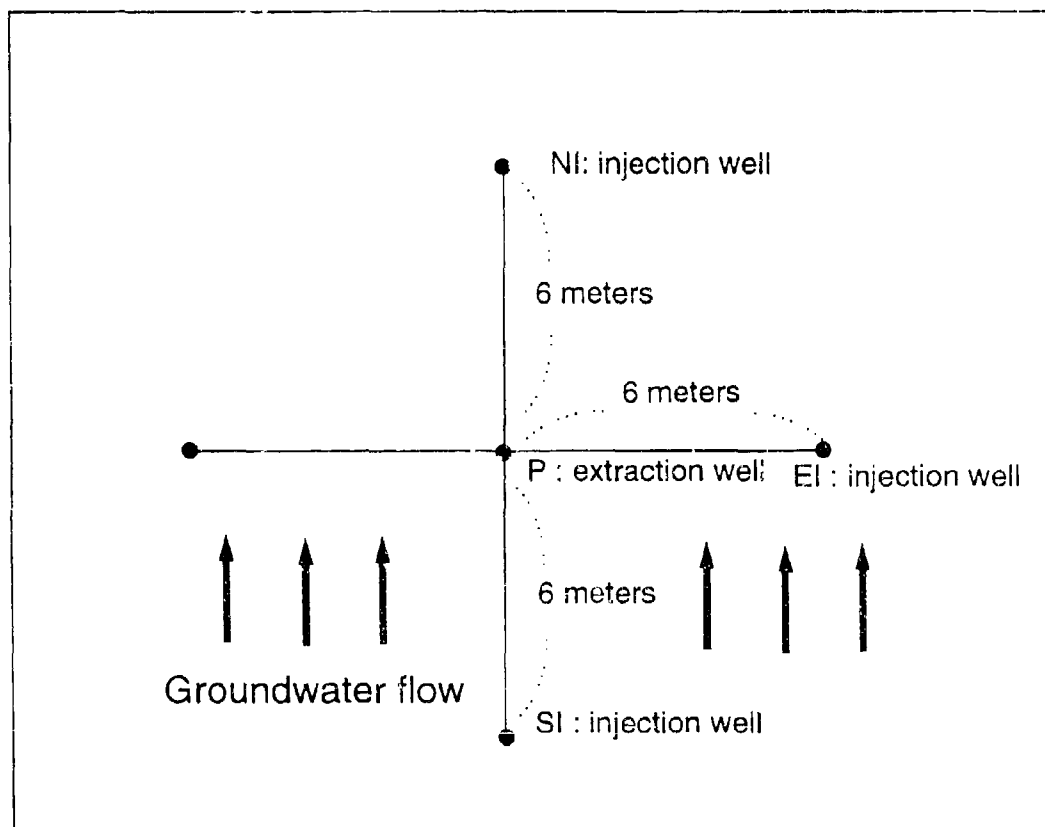


Figure 46. Map of the well fields installed at the field site.

Table 4. Input Data For RESSQ Example

Data 1:	Input	Explanation
1. Title	moffett	Field site at Moffett Naval Air Station
2. Number of injection wells (> 0)	3	To illustrate the original design of the well field
3. Number of production wells	1	One extraction well with higher flow rate to create an approximation of radial flow
4. Ambient concentration in aquifer	0.	Assume no background concentration
5. Default injection concentration	100.	
6. Units of concentration	(blank)	Blank (default) for using concentration in percentage
7. System of units	2	For practical units
8. Thickness of aquifer	1.2	Average aquifer thickness
Data 2:		
9. Porosity (percent)	35.	A porosity of 0.35
10. Pore water velocity	300.	A regional flow of 300 m/yr
11. Direction of regional flow	90.	Ground water flows toward the north
12. Adsorption capacity of rock matrix	0.	Assume no adsorption (retardation factor $R = 1$). Adsorption capacity $= 1 - 1/R$
13. Period of study	1.	Maximum amount of time for calculating the trace of a streamline (years)
14. Step length	1.	Spatial increment used to trace out streamlines (m)
15. Flag:plot of streamlines	-1	-1 suppresses plot of streamlines
16. Flag:plot of fronts	(blank)	-1 suppresses plot of fronts
Data 3:		
17. Number of fronts to be calculated around each injection well	7	(Maximum 7)
18. Time at which the 1st front is calculated	0.004	0.004 year = 1.46 day

19. Time at which the 2nd front is calculated	0.005	
20. Time at which the 3rd front is calculated	0.006	
21. Time at which the 4th front is calculated	0.007	
22. Time at which the 5th front is calculated	0.008	
23. Time at which the 6th front is calculated	0.009	
24. Time at which the 7th front is calculated	0.01	
Data 4:		
25. Minimum x for plot	-8.	Limit on the area studied (m)
26. Maximum x for plot	8.	
27. Minimum y for plot	-8.	
28. Maximum y for plot	8.	
Injection well 1:		
1. Name of the well	Injwell-1	Injection well SI
2. x coordinate of the well	0.	
3. y coordinate of the well	-6.	
4. Flow rate into the well	0.03	Fluid injection at a rate of 0.5 l/min (0.03 m ³ /hr)
5. Radius of the well	0.025	25 mm=0.025 m
6. Injection concentration	100.	
7. Angle at which the first streamline calculated leaves the well	0.	0. indicates positive x axis
8. Number of streamlines calculated for the well	30	
9. Ratio of number of streamlines to the number of streamlines plotted	3	
Injection well 2:		
1. Name of the well	inject-2	Injection well EI

2. x coordinate of the well	6.	
3. y coordinate of the well	0.	
4. Flow fate into the well	0.03	
5. Radius of the well	0.025	
6. Injection concentration	100.	
7. Angle at which the first streamline calculated leaves the well	0.	
8. Number of streamlines calculated for the well	30	
9. Ratio of number of streamlines to the number of streamlines plotted	3	
Injection well 3:		
1. Name of the well	inject-3	Injection well NI
2. x coordinate of the well	0.	
3. y coordinate of the well	6.	
4. Flow fate into the well	0.03	
5. Radius of the well	0.025	
6. Injection concentration	100.	
7. Angle at which the first streamline calculated leaves the well	0.	
8. Number of streamlines calculated for the well	30	
9. Ratio of number of streamlines to the number of streamlines plotted	3	
Production well 1:		
1. Name of the well	Prodwell-1	Extraction well P
2. x coordinate of the well	0.	
3. y coordinate of the well	0.	
4. Flow rate from the well	0.48	Extraction rate of 8 l/min (=0.48 m ³ /hr)
5. Radius of the well	0.025	

6. Flag: to suppress study
concentration

of (blank)

Blank means production concentration is to be
studied

The results (see Figure 47) indicate that it is advantageous to use the southern leg for the bioremediation experiments. The reasons are the following: (1) the injected fluid supplying the nutrients becomes less dispersed, and hence a more dense microbial population can be stimulated; (2) by injection upgradient, the injected tracers and chlorinated hydrocarbons can be most effectively recovered at the extraction well.

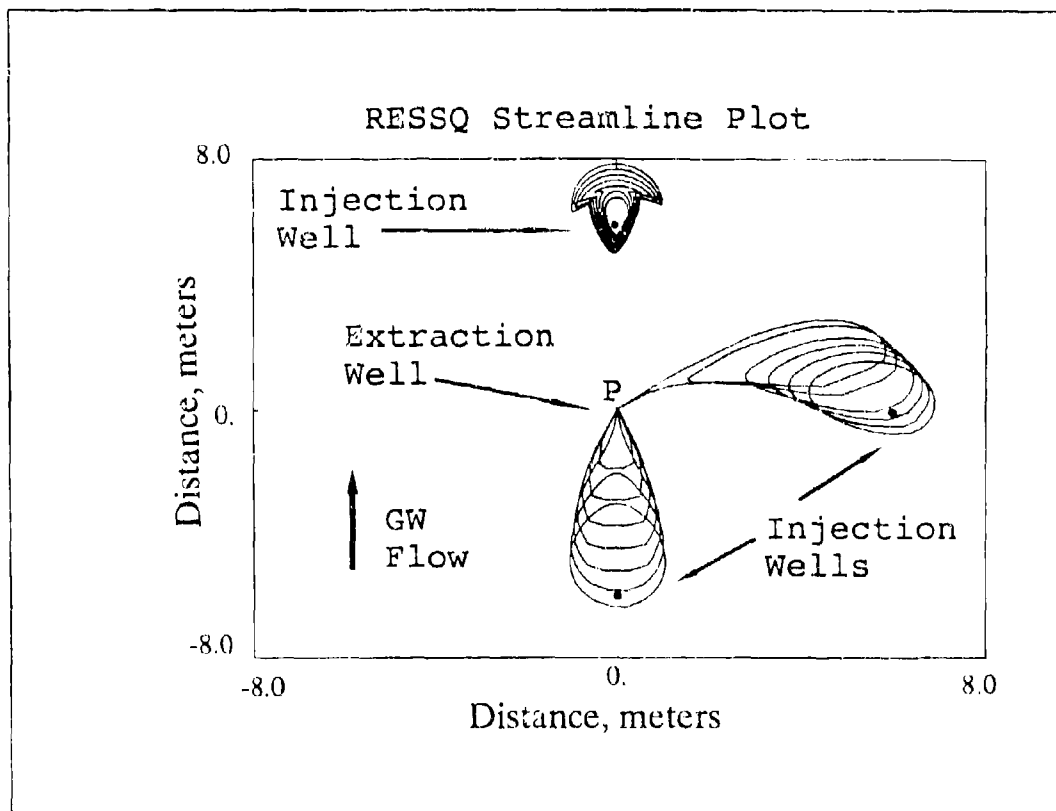


Figure 47. RESSQ Streamline Plot for Moffett Base

3. Example Three: USGS MOC

The two-dimensional flow and mass transport numerical model, MOC, was used to simulate groundwater transport within the OU 3, Hill AFB, Utah. This model has been updated for simulating the transport of non-conservative contaminants. The area of the regional model comprises all the potential sources in OU 3 and a substantial area downgradient of OU 3. The model consisted of uniformly spaced cells at 250-foot intervals with 38 columns and 39 rows. All recharges, discharge, and leakage was determined for each cell based on flow conditions established by the regional groundwater flow model MODFLOW. Values used for permeability and aquifer thickness and other hydrologic properties were the same as the regional groundwater flow model.

The preprocessor program PREMOC can be used to view the input file, HILL109.dat, which is quite lengthy and is provided with the software package. An isoconcentration map of predictions is provided below (Figure 48): contour interval from 1 $\mu\text{g/l}$ to 21 $\mu\text{g/l}$, retardation factor $R = 1$, concentration in $\mu\text{g/l}$.

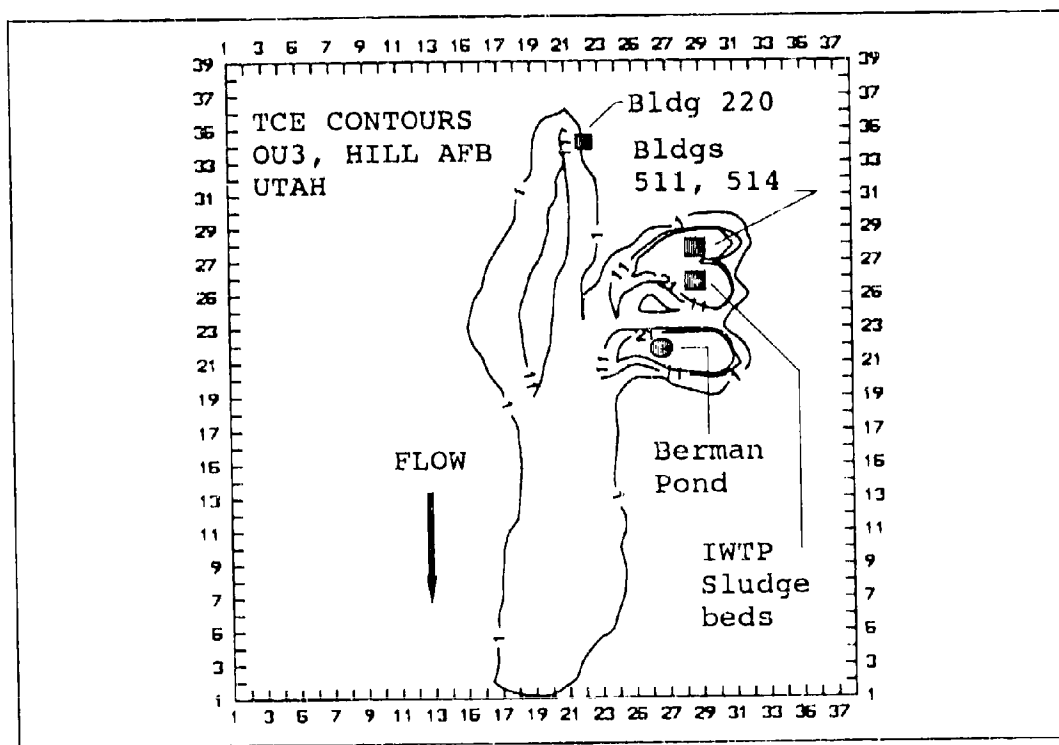


Figure 48. TCE Contours for Operable Unit 3, Hill AFB

Figure 49 is a three-dimensional view of the simulated TCE concentration contours. The authors have visited the site twice and obtained extensive data from Hill AFB Installation Restoration staff.

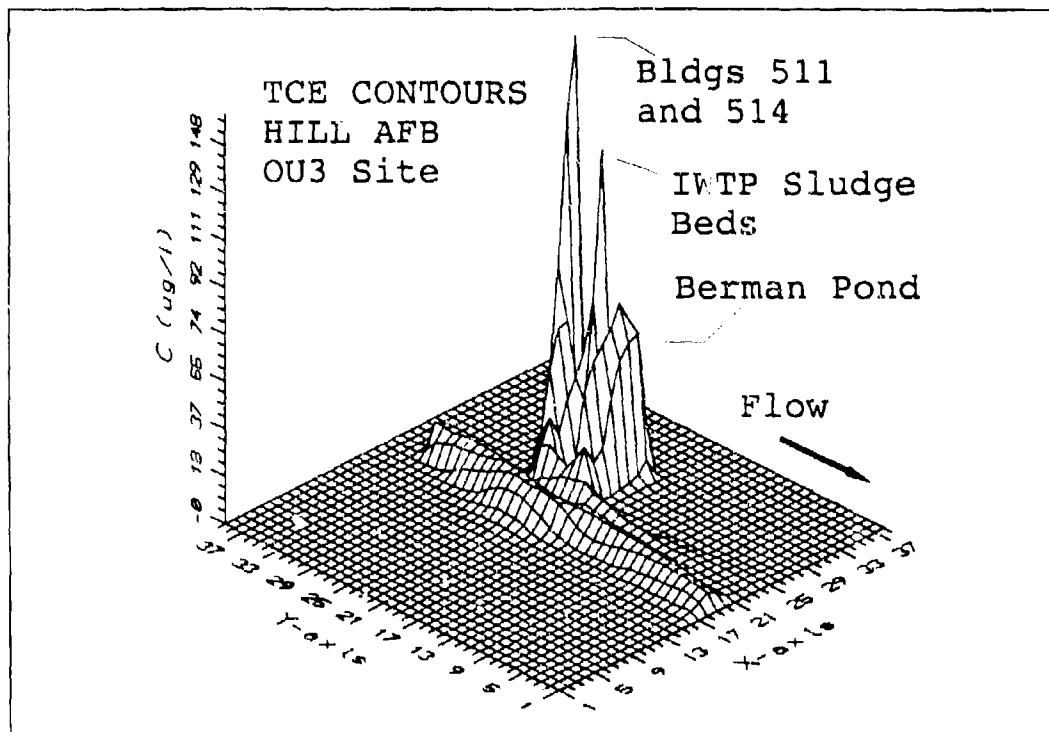


Figure 49. TCE Concentration Surface, Hill AFB OU3

4. Example Four: ODAST in Monte Carlo mode

The one-dimensional analytical model ,ODASTMC , was developed to account for uncertainty in the simulated concentration. This example also uses data from OU 3 (Operable Unit 3, Hill Air Force Base, Utah). In Monte Carlo simulation, the input parameters are assumed to be random variables. After repetitive executions of the model, it will generate an output probability distribution associated with the contaminant concentration at the point of interest. In this example, the point of interest is monitoring well ESE-6 which is 2350 feet from the contaminant source (near monitoring well ESE-9). The observed concentration at ESE-6 in 1991 was 4.9 $\mu\text{g/L}$. The simulated mean concentration is 6.156 $\mu\text{g/L}$. Table 5 summarizes the input data.

Table 5. Input Data for ODASTMC

Data 1:	Input	Explanation
1. Number of x positions	6	Assume source of TCE located at monitoring well ESE-9. The 6 x positions are southwest from the source.
2. 1st value of distance (x) from the source	304.8	304.8 meters=1000 feet
3. 2nd value of x	609.6	609.6 meters=2000 feet
4. 3rd value of x	717.2	717.2 meters=2350 feet (location of monitoring well ESE-6)
5. 4th value of x	1219.2	1219.2 meters=4000 feet
6. 5th value of x	1524.0	1524.0 meters=5000 feet
Data 2:		
1. Number of time points	5	Sources released from 1940
2. First value of time at which concentration is evaluated	10.	Year 1950
3. Second value of time at which concentration is evaluated	20.	Year 1960
4. Third value of time at which concentration is evaluated	30.	Year 1970
5. 4th value of time at which concentration is evaluated	40.	Year 1980
2. 5th value of time at which concentration is required	51.	The elapsed time is 51 years. The time at which concentration is evaluated is 1991.
Data 3:	MV SD PDT	MV= mean value, SD= standard deviation, PDT= parameter distribution type (1: uniform distribution; 2: normal distribution; 3: log normal distribution)
1. Time of waste recharge	36. 0. 2	A source released contaminants to the ground water for 36 years (1940 to 1976)
2. Pore water velocity	0.0835 0.00835 2	(1) Groundwater velocity= 100 ft/yr = 0.0835 m/day (2) From slug test results, most of the velocities were less than 100 ft/yr.

3. Longitudinal dispersivity	60.96 6.096 2	Dispersion coefficient = velocity x dispersivity
4. Diffusion coefficient	0. 0. 2	molecular diffusion
5. Source concentration	150. 15. 2	$\mu\text{g/L}$
Data 4:	MV SD PDT	MV= mean value, SD= standard deviation, PDT= parameter distribution type (1: uniform distribution; 2: normal distribution; 3: log normal distribution)
1. Bulk mass density	1.99 0.199 2	g/cm^3
2. Porosity	0.25 0.025 2	
3. Distribution coefficient	0.44 0.044 2	$R = (1 + K_d \rho_b) / \phi$ R= retardation factor ρ_b = bulk mass density K_d = distribution coefficient ϕ = porosity
4. Radioactive decay factor	0. 0. 2	
5. Decay factor of the source	0. 0. 2	
Data 5		
1. Target concentration to evaluate	5.	Maximum allowable concentration ($\mu\text{g/L}$)
2. Number of Monte Carlo Runs	1000	
3. Observation point of X	3	X position where potential human exposure is evaluated (check Data 1.)
4. Observation point of T	5	Time point where potential human exposure is evaluated (check Data 2.)
5. Name of contaminant	TCE	

6. Name of site

Hill

The input file for: MODEL.DAT is

```
8 5
304.8 609.6 717.2 914.4 1219.2 1524.
10. 20. 30. 40. 51.
36. 0.2
0.0835 0.00835 2
80.96 6.096 2
0. 0.2
150. 15.2
1.99 0.199 2
0.25 0.025 2
0.44 0.044 2
0. 0.2
0. 0.2
5. 1000 3 5 TCE Hill
```

The output file for ODASTMC: MODEL.OUT is

```
TIME = 10:22:38.28
TIME = 10:22:49.87
Elapsed time: 1159E+02 seconds
```

The number of Monte Carlo run: 1000

The mean values of parameters:

SOURCE CONCENTRATION C0 = 150.00

V= .08 D= 5.09 R= 4.50 LAMBDA= .000 ALPHA= .000 T0= 36.0 T(YEARS)

The observation point: X= 717.200 T= 51.000

The mean value of concentration: 8.156

The standard deviation of concentration: 5.785

The concentration for evaluation: 5.000

The probability of failure: .454

The distance-time matrix is:

T	X
10.0000	304.8000 609.6000 717.2000 914.4000 1219.2000 1524.0000
20.0000	304.8000 609.6000 717.2000 914.4000 1219.2000 1524.0000
30.0000	304.8000 609.6000 717.2000 914.4000 1219.2000 1524.0000
40.0000	304.8000 609.6000 717.2000 914.4000 1219.2000 1524.0000
51.0000	304.8000 609.6000 717.2000 914.4000 1219.2000 1524.0000

The probability of failure matrix is:

0020	0000	0000	0000	0000	0000
8780	0000	0000	0000	0000	0000
10000	0180	0000	0000	0000	0000
10000	3890	0530	0000	0000	0000
10000	8690	4540	0180	0000	0000

The predicted cumulative distribution function is shown in Figure 50.

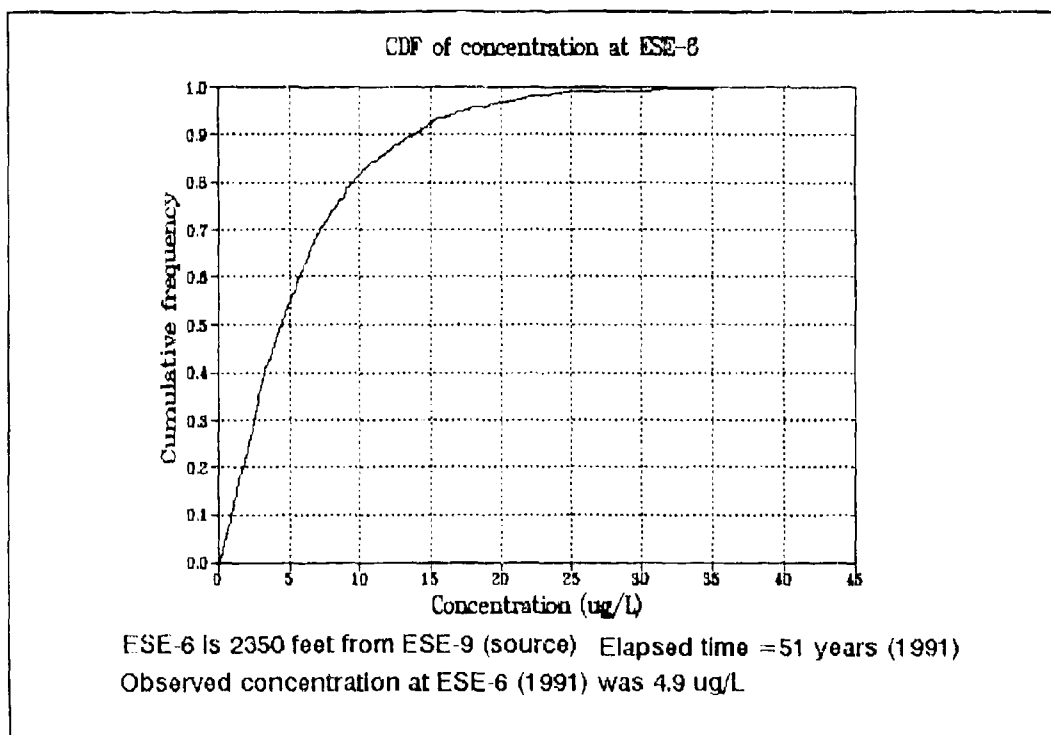


Figure 50. Predicted Cumulative Distribution Function for TCE

SECTION IV

USERS GUIDE FOR THE UNIX VERSION

This section provides a detailed guide to the use of the Advisory System in the UNIX environment. As with the DOS version of the Advisory System, the intended audience is a user reasonably familiar with the general theory of contaminant transport in porous media, and the UNIX operating system. However, the user may not have experience with a particular transport model. This section contains a generic guide to the Advisory system, generally applicable and independent of the specific contaminant transport model. The generic guide to the Advisory System includes subsections A,B and C. The subsequent sections present more detailed information on the specific models in the UNIX version of the Advisory System that have some differences (even though minor in some cases) from the DOS version.

For each model, notes are provided on the applicability of each model, the inherent limitations of a particular modeling approach, data preparation and output. Section III(G) presents four applications of specific models within the Advisory System, which are identical to the UNIX version.

A. STARTING THE SYSTEM

This section assumes that the Advisory System has been properly installed on the UNIX-based workstation according to the instructions provided in Section II(B). To start the Advisory System, switch to the sub-directory "gwadv" and execute the command "gwadv". An introductory screen for the Advisory System, which identifies the version, appears (see Figure 51).

B. FILE MANAGEMENT

The first task is to identify the site for study and establish the needed data files. Another screen presents the user with a list of the LEVEL 0 options. Option 1 provides a simple introduction to the system. Option 2 provides access to a previously analyzed site. Choosing this option will locate and access all existing files dealing with the site. Option 3 allows the user to analyze a new site. The Advisory System will automatically check that files with the user-supplied names do not already exist. The user is prompted with appropriate alternatives if the files already exist. Option 4 terminates the Advisory System and Option 5 allows the user to proceed directly to LEVEL 1 of the system (Figure 52).

For a previously analyzed site, the user is prompted for a 7-character file name which includes the site name and model ID. The site name and model ID should consist of 5 letters and 2 numerical digits, respectively. Together, the site name and model

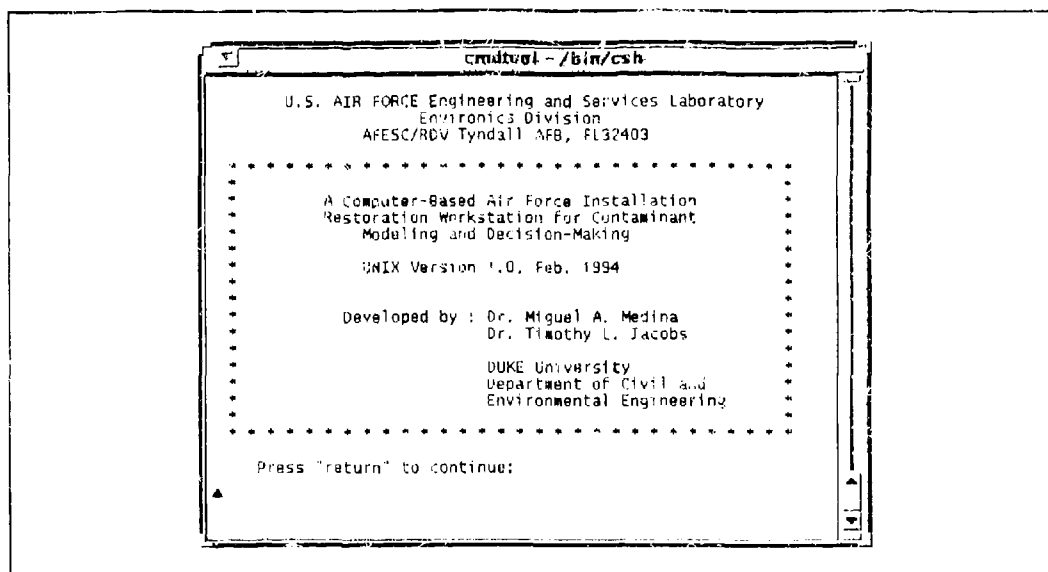


Figure 51. Advisory System UNIX Introductory Screen

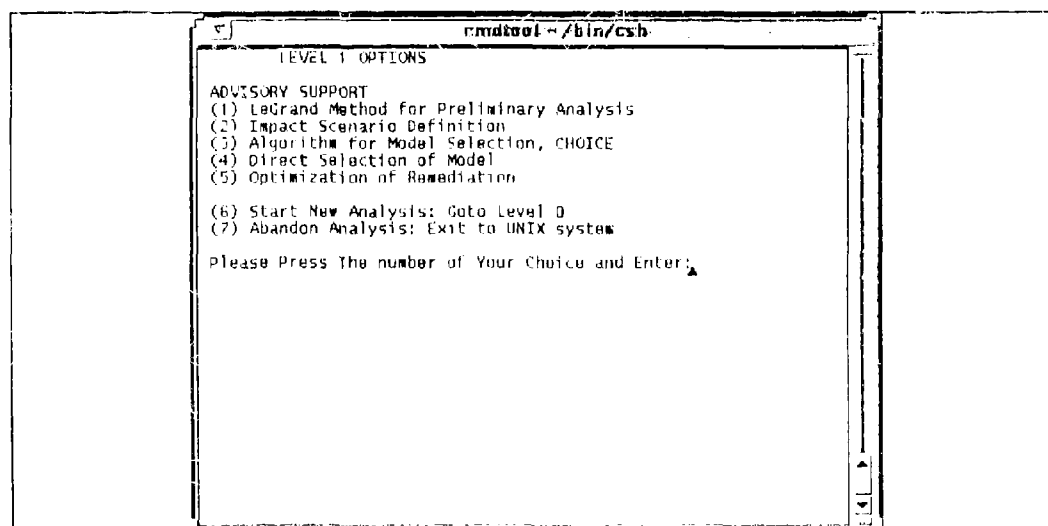


Figure 52. Level 1 Options, UNIX Version

ID identify the files associated with the site, and the specific model previously applied to the site analysis. For example, Figure 53 below illustrates the screen display for a previously analyzed site.

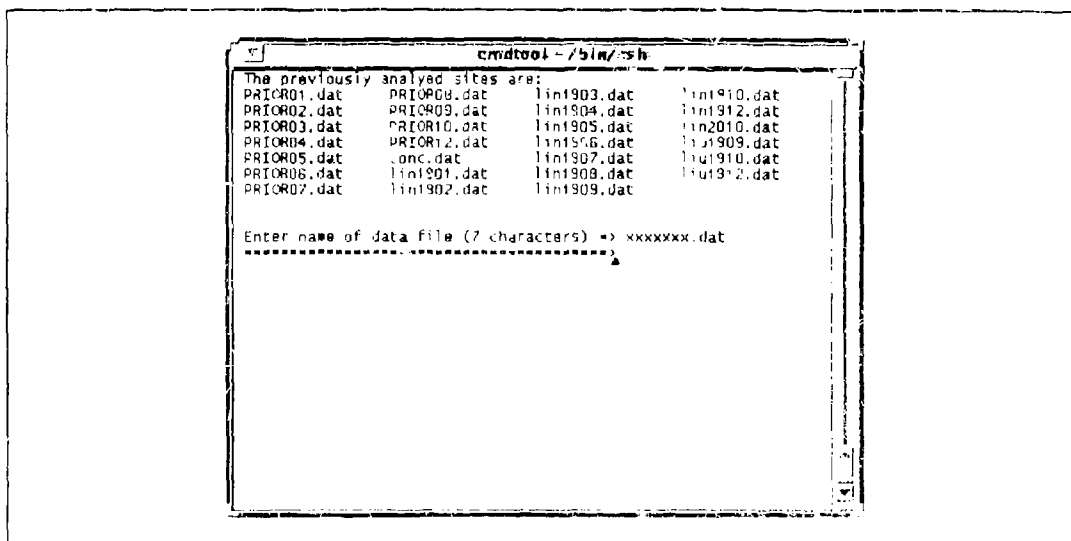


Figure 53. Screen for previously analyzed site files

To analyze a new site, the user selects Option 3 and is prompted for a 5-character site and a header identifying the analyst, date and title of the project. With completion of this step, the Advisory System proceeds to the LEVEL 1 menu. This option can also be used to re-analyze a previously analyzed site.

For users not experienced with the Advisory System, Option 5 allows the user to proceed to the LEVEL 1 menu using the default site name "PRIOR" to create the necessary input and output files.

C. LEVEL 1, MASTER MENU

After setting up the necessary files, the system proceeds to the LEVEL 1 menu. LEVEL 1 controls all pathways to the system and is accessed by the LEVEL 1 MASTER MENU (Figure 52 shown earlier). Level 1 options are divided into two categories: "Advisory Support" and "File Utilities." The utilities are self explanatory and helpful for file management. The option of advisory support provides access to either preliminary analysis, or all the transport models within the Advisory System.

D. PRELIMINARY ANALYSIS

In many cases, it may appear to the analyst that a site is so poorly situated that detailed modeling cannot be used. In other cases, some sites may need preliminary

analysis to evaluate the hydrogeology and provide a guide to further data collection. To formalize this subjective process, the Advisory System provides a preliminary analysis using the LeGrand method. In most cases, the LeGrand method should be the first step in the analysis process (Option 1 of the Level 1 Menu).

In the early stage of a site investigation, project managers usually lack the resources to conduct a detailed modeling analyses of all sites potentially affecting the groundwater. Due to poor hydrogeological conditions, it is often necessary to perform a preliminary investigation to guide further site investigation. Conversely, some cases will have such a low degree of contaminant severity and potential risk of contamination that a site could be assessed without detailed modeling. Often, the decisions concerning the site modeling are subjective in nature. However, it is safer and beneficial to establish a formal mechanism for deciding on how a specific site should be modeled.

The criteria and methodology used to perform the preliminary analysis in the UNIX version of the Advisory System is identical to that used by the DOS version of the system. For a detailed discussion of the LeGrand method, please refer to Section III(D).

E. ACCESS TO MODELS

The Advisory System provides the user with two methods for accessing the models within the system. The first method involves the CHOICE algorithm which provides a formal mechanism for selecting the appropriate groundwater model with respect to the available site data. The second method involves the direct selection of a specific groundwater model. This approach allows users with extensive experience in groundwater and contaminant transport modeling to bypass the model selection routine. The following sections provide detailed descriptions of selected models only as noted above. The CHOICE algorithm in the UNIX version is identical to that of the DOS version; for specific details regarding its operation and use, please refer to Section III(E). The direct selection of models within the system is self-explanatory and menu-driven for user convenience.

F. INPUT/OUTPUT DATA FORMATS FOR SPECIFIC MODELS

The UNIX version of the Advisory System uses Open Windows version 2.1.1 to access, edit and process the input and output data for all the models in the system. In addition, the windowing software allows the user to view both input and output information simultaneously. The window drivers are all automatic and provide the user with easy access to any files within the system. Figures 54 and 55 illustrate the accessibility of both input and output files used by the system. The actual use of these windows is very simple and self-explanatory. If you are not familiar with the use of the Open Windows system, familiarize yourself by experimenting with the creation, editing

and saving of temporary files before you start running the Advisory System. If you have any questions concerning the *Open Windows* system, please consult the users manual included with the workstation.

Graphics output for the system is similar to that of the standard input and output files. Whenever the user selects a graphical mode for the presentation of modeling results, the Advisory System automatically forks a new window using the *Open Windows* software and displays the desired output. These windows can be deleted or saved using the standard windowing options available in *Open Windows*. A word of **caution**: you should never try to display an executable file while running the Advisory System. Doing so may cause the window to "freeze", resulting in a great deal of aggravation. In addition, you might accidentally corrupt the file which will prevent it from working properly.

parameters	mean	variance	type
Longitudinal dispersion coefficient, m^2/d	1.0000	0.1000	2
Transverse dispersion coefficient, m^2/d	0.1000	0.0100	2
Pore water velocity, m/d	0.1000	0.0100	1
Half length of source, m	50.0000	5.0000	3
Radioactive decay factor, $1/d$	0.0000	0.0000	0
Retardation factor	1.2000	0.0100	2
Decay factor of the source, $1/d$	0.0000	0.0000	0

Figure 54. A screen for access to input data

In the following sub-sections suggestions are provided on the use of component models in the system, following the same format as in the DOS section. In each case, the following items are addressed: 1) applications of the particular model, 2) limitations of the model's approach, and 3) details of data input and output for specific models.

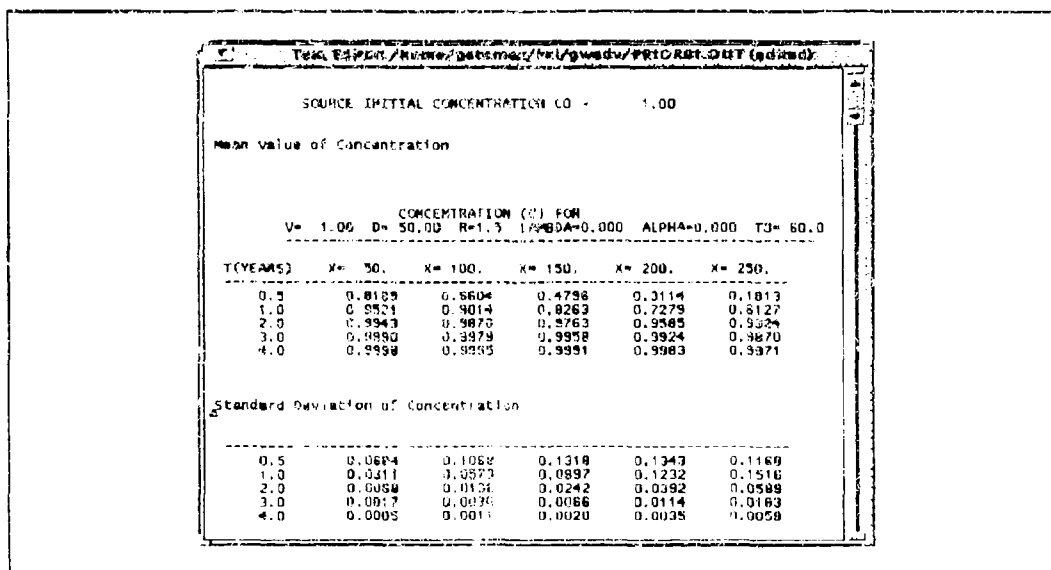


Figure 55. A screen for access to an output file

1. ODAST

The program ODAST evaluates the one dimensional analytical solute transport solution considering convection, dispersion, decay and adsorption in porous media (Javandel et al., 1984). The program has been modified to facilitate Monte Carlo analysis. The solution method handles many types of transport conditions, and is also numerically stable and computationally efficient. The idealized situation from which the solution arises is as follows: the model considers an infinitely long column of a homogeneous isotropic porous medium with a steady state uniform flow of constant seepage velocity. A particular solute is injected from one end of the system for a period of time such that the input concentration may vary as an exponential function of time. The value of concentration may then be calculated at any time t and distance x from the injection boundary. In the field, such an idealized situation could be represented by an infinitely long ditch of contaminated waste water fully penetrating an infinitely long confined aquifer, with the ditch cutting the aquifer perpendicular to the direction of flow.

The idealized situation described obviously does not exist in the real world. However, the solution provides a valid approximation in many cases. As with most analytical solutions the assumption is made of isotropic, uniform, steady state regional flow. This will often be a reasonable approximation of actual flow conditions. Likewise, the

assumption of a confined aquifer may provide a reasonable approximation for analysis of phreatic aquifers if the flow regime is not strongly altered by the rate of fluid input from the source, and the saturated thickness remains approximately constant. Even where the saturated thickness is to some extent variable over time use of the average saturated thickness will enable analysis of average contamination risk. This approximation will be particularly valid for analysis in the Monte Carlo mode. In the Monte Carlo mode the input concentration and regional flow velocity both become random variables, and the cumulative frequency estimated over these and other random parameters should provide a reasonable estimate of the average risk. If however the source itself contributes fluid that becomes an important factor of the flow regime, so that radial flow from the source is established, the confined aquifer assumption becomes inappropriate, and the phreatic surface will move in response to the source input. This condition is tested for in the CHOICE algorithm. Another model, DUPVG, may be appropriate under these conditions.

Obviously, real sources will not be of infinite length. However, the one dimensional solution provides a reasonable approximation for finite sources if the observation point is sufficiently near the finite width source so that the effect of the source edges will be minimal. For instance, if a source has a lateral extent of 200 feet and the perimeter of compliance is 50 feet from the source, the one dimensional solution is likely to provide a reasonable (and conservative) approximation of contamination risk along the axis extending from the center of the source (but not near the source edges). The exact distance to which the one dimensional solution can be carried downstream from a finite source without introduction of unacceptable error will depend on the interaction of all the forces controlling the flow regime.

The method can also be extended to cover input configurations other than the ideal ditch perpendicular to flow. Many situations of interest will involve large areal surface applications of wastes. Modeling the actual distribution of contamination in such cases is a complex process. However, solutions such as ODAST may be appropriate given certain assumptions. The first step is to calculate the rate of mass loading at the water table surface, after any vadose zone attenuation. We must then make the assumption that the substance is more or less instantly vertically mixed in the aquifer. Such an approximation is of course more valid for relatively thin surficial aquifers. (Generally, when the degree of vertical penetration is a significant factor in determining plume development, a three-dimensional solution, such as EPAGW, must be employed.) This constant areal input must then be represented as a line source at the downflow edge of the area. To do this one can make the simplifying assumption that the whole aquifer volume beneath the landfill is thoroughly mixed by the time flow reaches the downstream edge of the source, and calculate an edge concentration based on the loading diluted by the regional flow. (The concentration at the edge of the aquifer will thus have a maximum possible value equal to the leaching concentration.) Such an approach is most applicable where the loading is approximately constant over the whole area. (An alternative is to model the areal source as a Gaussian source, maximum at the center and declining towards the edges. This option is provided by EPAGW.) Model input

provides options for calculating concentration in this manner, or for direct input of the concentration at the source edge.

The nature of the solution, and the additional assumptions that may be needed to employ it, as indicated above, introduce a number of **limitations** in the applicability of the model. First, ODAST is clearly inapplicable when the source cannot be modeled as laterally approximately infinite in terms of the point of interest. As with all analytical solutions, the model will not be appropriate where there is a significant deviation from the conditions of uniform, steady-state regional flow. However, minor violations of these conditions will not have important effects on the general analysis of contamination risk, and the model will also be valuable for initial analysis when non-uniform flow is suspected, but not fully documented. The solution also assumes a semi-infinite flow regime, and thus cannot take into account aquifer interactions with constant head boundaries, such as rivers. The CHOICE algorithm suggests avoiding use of this type of analytical solution when the perimeter of compliance or other point to be modeled is within 250 feet of a fixed head boundary. Limitations that are more difficult to assess involve the assumptions that vertical concentration gradients can be ignored (full mixing), and that the source can be modeled as a uniform strength line. Clearly, the solution cannot be used for liquid contaminants that are not fully miscible and tend to float or sink within an aquifer. Further, ODAST may result in underestimation of contaminant risk at the aquifer surface if full mixing does not occur.

The preprocessor developed for ODAST follows a standard format that is used for most of the models in the system. This consists of presentation of a number of screens, with input slots to be filled. The user has to key in the required input data with the same format shown on the screen. An error-detection design in the preprocessor provides the user a opportunity to go back to the same screen if he/she has made any mistake. Input data for ODAST includes the followings:

NUMX: Number of points modeled in the X direction, which establishes the 1-dimensional grid. From 1 to 25 points may be used. Grid size does not affect solution, and for Monte Carlo simulation you will normally wish to examine only one or two points at the perimeter of compliance in order to speed execution. The X direction is coincident with the regional flow vector.

NUMT: Number of time steps for calculation. In Monte Carlo applications only the last time step will be tabulated for cumulative frequencies. However, the output file will contain sample data from each time step. In deterministic mode full data will be provided for each time step.

MONTE CARLO MODE: In Monte Carlo applications, the user needs to input the probabilistics of the random parameters, including their mean, variance and type of probability distribution. Three options are available in the Advisory System. Type=(1) generates values of parameters as an uniform distributions by use of Box-Muller method.

With option Type=(2), normal process is used. With Type=(3), log-normal distribution is adopted.

DL: Longitudinal dispersion coefficient. In deterministic mode, or in Monte Carlo mode For MC the mean and standard deviation of dispersion coefficient are required

V0: Mean pore water velocity of the regional flow, required input for either deterministic mode or Monte Carlo mode. This can be estimated from the average observed flow velocity, v , as $V0=v/P$, where P is the porosity of the medium.

ALAM: The "radioactive" decay factor of the contaminant in the saturated medium.

$$ALAM = \frac{\ln 2}{HL} \quad (18)$$

where HL is the half-life (days). Note that ALAM can be used to represent chemical hydrolysis by entering the generalized hydrolysis rate as ALAM. Specify ALAM=0. for no decay or hydrolysis. Hydrolysis rates typically vary with pH and can be estimated from acid, base and neutral rate constants (K_{hao} , K_{hbo} and K_{hno}). The generalized hydrolysis rate constant, K , can then be approximated by the relationship (Mulkey and Brown, 1985):

$$K = \frac{K_{hbo} [OH^-] \theta + (10 K_{hao} [H^+] + K_{hno}) \beta \rho_b}{\theta + \beta \rho_b} \quad (19)$$

for rates expressed in days⁻¹, in which $[H^+]$ is the hydrogen ion concentration, M, equivalent to $\exp(-pH)$; $[OH^-]$ is the hydroxyl ion concentration, where at equilibrium in water $[OH^-][H^+] = 1.0 \times 10^{-14}$; β is the soil-water distribution coefficient (see next section); θ is the volumetric water content of the soil (total porosity for saturated media), and ρ_b is the soil bulk density as g/cm³. In equation (19), the term $K_{hbo} [OH^-]$ represents the first-order hydrolysis rate for the dissolved constituent. Where K is not known this term may be replaced by $K_{hbo} [OH^-] = (K_{hao} [H^+] + K_{hno})$. The rates can be altered to additionally reflect biodegradation and volatilization where information is available. Total rates may also be directly estimated from an observed half life (HL) as $ALAM = \ln 2 / HL$. Rates are 1/days.

R: retardation coefficient, $= v/v_c$, where v is the velocity of the regional flow and v_c the apparent velocity of the contaminant. If we assume reversible linear adsorption, R can be estimated as:

$$R = 1 + \frac{\beta \rho_b}{\theta} \quad (20)$$

For this model, soil bulk densities are not explicitly considered, and the user must input a computed value for R . However, for the typically encountered ranges of porosities and soil bulk densities R , can be approximated as falling within a limited range (Freeze and Cherry, 1979):

$$(1 + 4\beta) \leq R \leq (1 + 10\beta) \quad (21)$$

The value of β will also vary with the type of the medium, particularly the organic carbon fraction of the soil. Values of β are typically reported as K_{oc} , where K_{oc} is the distribution coefficient normalized to organic carbon. In the case where hydrophobic binding dominates the sorption process, the actual distribution coefficient can then be estimated by:

$$\beta = f_{oc} K_{oc} \quad (22)$$

where f_{oc} is the fraction of organic carbon in the soil. Values of f_{oc} are not widely available, but are generally thought to lie in the range of 0.001 to 0.01 for most soils (Mulkey and Brown, 1985). For other binding mechanisms this relationship cannot be used (see Karickhoff, 1985).

ALFA: Similar to ALAM, but represents the rate of decay of the source strength. Specify ALFA=0, for constant source strength.

T_0 : Total time period of waste recharge in years.

The output of ODAST has two formats:

(1) Text format - the UNIX version of Advisory System provides a text editor window which allows the user to view, edit and store the output data for later use.

(2) Graphics format - there are eight options for the user to see the contaminant concentration on the time-distance domain;

- a. time-distance grids plot,
- b. monochrome contour,
- c. monochrome contour with grids,
- d. colors contour,
- e. grey-tone contour,
- f. full color contour,
- g. vector plots,
- h. perspective plot.

2. TDAST

The model TDAST evaluates the two-dimensional solute transport case with an analytical solution, considering convection, dispersion, decay and adsorption in porous media (Javandel et al., 1985). The idealized conception of the model is related to that of ODAST, but covers another important class of cases. As with ODAST we assume conditions of steady-state, uniform flow in a confined aquifer. The source is again assumed to be fully penetrating, but in this case is of finite lateral extent (normal to flow), as in the case of a fully-penetrating ditch of finite length. Thus, TDAST is applicable in conditions similar to those applicable for ODAST, except that here the observation point is far enough from the source boundary so that the effects of the source edge and transverse dispersion must be taken into account in the approximation. By using the same techniques as described above for ODAST, TDAST may be applied to constant areal waste sources. In such a case, ODAST would be accurate for analysis near to the center of the source edge, while TDAST could be used for such a location and also locations nearer to the source edge, and locations further away from the source boundary. In general, the numerical stability and speed of ODAST make that solution preferable where applicable. TDAST is also useful for analysis of contamination resulting from smaller sources.

The same general **limitations** apply to TDAST as apply to ODAST, except that the effects of lateral source geometry and transverse diffusion are explicitly considered. That is, the approximations of full penetration (vertical mixing) and uniform, steady state flow must also be met here. TDAST also assumes that the source is aligned normal to the regional flow, although the solution could readily be altered to take into account other geometries. An important practical limitation of the present version of TDAST arises from its use of a numerical technique to evaluate an integral. Presently TDAST uses a Gauss-Legendre polynomial method for this evaluation, making use of the same subroutine employed in the models EPASF and EPAGW. The number of terms in the polynomial evaluation may be set by the user, up to a certain limit. The solution routine begins with a lower number of terms and increments the number until the solutions converge (within 1%), or the limit is reached. Under certain conditions adequate convergence cannot be achieved within the limits available in the numerical integration scheme, which will result in the display of a warning message. In general, lack of convergence will be encountered when the ratio of Vt/X becomes much greater than 1 (where V is velocity, t is time and X is distance). This means that TDAST provides accurate calculation of the time period during which concentration increases at a given point, as the plume breakthrough occurs, but loses accuracy at a given point as time increases past breakthrough, resulting in underestimation of concentrations. However, this is merely an inconvenience for analysis, as the solution should approach a steady-state concentration before numerical instability overwhelms the solution. The user should thus fine-tune the application to avoid this problem. This can be done for the desired time step by eliminating those observation points that are well behind the

breakthrough curve of the plume. As noted above, because of convergence problems in the estimation of the integral, it is not practical to specify observation points very near the source as time increases. However, the user may always include points at $X=0$. At this point the concentration will simply be given as the calculated source concentration interpreted as a line source at the boundary.

The data input is essentially the same as that for ODAST, described above, with the addition of the following variables:

NUMY: Number of Y positions in the grid. Observations will be calculated at all combinations of NUMX, NUMY and NUMT.

NNS: This sets the accuracy of the numerical integration scheme used by TDAST, by choosing the degree of the polynomial for the Gauss-Legendre method. NNS selects the nth digit from (4, 5, 6, 10, 15, 20, 30, 40, 50, 60, 104, 256). Increasing NNS improves accuracy but decreases speed. $NNS=8$ seems to provide a good compromise value with which to start, but may be changed at will. If convergence warnings appear on screen during run time the user should try increasing the value of NNS.

DT: Transverse dispersion coefficient. As in ODAST, the dispersion coefficients must be input for deterministic modeling, but can be estimated from scale and velocity in Monte Carlo mode. In the latter case DT is estimated as $1/3$ of DL.

A: Half-length of the source, being $1/2$ of the lateral extent of the source normal to the direction of flow.

The output formats are similar to that of ODAST, except that the concentration contours are on the $x - y$ space domain.

3. PLUM2D

The model PLUM2D is an analytical model for calculation of the tracer concentration distribution in a homogeneous, nonleaky confined aquifer with uniform regional flow. The solution method is based on the Hantush Well-function, in which the Well-function flow solution for a leaky confined aquifer is applied by analogy to account for transport and dispersion in a nonleaky confined aquifer. Source strengths are assumed constant, but the solute may be subject to adsorption and radioactive type decay in the porous medium.

An important advantage of this method is that it can readily treat multiple point sources, which sources may have been operational for differing amounts of time. This enables PLUM2D to treat certain situations that cannot be handled by other analytical methods. The solution is based on an idealized situation, in which solute is introduced

into a fully homogeneous confined aquifer through one or more fully penetrating wells in the presence of regional two dimensional, horizontal ground water flow. The injection rate from these wells is considered to be sufficiently small that it does not alter the regional flow pattern. Thus the model is most applicable to injection wells with relatively low injection rates. However, PLUM2D can provide a reasonable approximation for other situations as well. That is, surface sources can be modeled as fully penetrating sources if the assumption is made that the solute is fully mixed in the vertical direction soon after its introduction into the aquifer. Further, the solution method is approximately appropriate for use in a surficial aquifer, when the saturated thickness is relatively constant, and the leaching rate from the sources is of a small enough magnitude such that it does not affect the regional flow regime through mounding.

In incorporating the model into the system we have provided a complete preprocessor and equipped the model for Monte Carlo simulation. In order to account for the correlation of the various parameters controlling the regional flow regime these are generated from simpler, underlying variables (see discussion of EPAGW for more details). However, a user option is also provided in Monte Carlo mode for direct input of hydraulic conductivity and dispersion values.

As with many of the other two-dimensional analytical models incorporated into the system, use of PLUM2D is **limited** to cases where it is reasonable to model the aquifer as if it were a confined aquifer with fully penetrating sources. These sources are treated as point sources, and thus the model is applicable to areal sources only where these can be treated as clusters of point sources. The model further assumes that source strength is constant, once initiated, and cannot handle situations in which the strength of the source is decaying over time.

As with most models in the system, we have provided a standard format preprocessor for PLUM2D. The user is provided with an option to specify input in either metric units [m, day] or English units [U.S. gallon, ft., day]. Data input is as follows:

UNITS: User option to select English or metric units.

TITLE: Title to be used for output.

NPTS: Number of solute injection wells specified, or other sources that can be approximated as injection wells. Up to 10 may be used in the present configuration of the model.

NOBS: Number of observation points for Monte Carlo simulation (up to 5). These are the points at which cumulative concentration frequencies will be calculated, and are in addition to the gridded calculation of concentration. For deterministic mode this variable is not needed.

NX: Grid dimension for calculation, number of nodes in x-direction. As this is an analytical solution, for Monte Carlo simulation a very sparse grid may be specified if interest is in only the frequency of concentrations at the observation points, rather than plume development. Specifying a sparse grid will greatly speed execution. The X axis is assumed to be coincident with the direction of regional flow. NX can range from 2 to 20.

NY: Grid dimension for calculation, number of nodes in y-direction. Range 2-20.

IRAD: User option to include radioactive decay (1=yes, 0=no). As in other models, decay processes such as hydrolysis can often be modeled as radioactive decay, if an effective "half-life" can be established. PLUM2D does not include the ability to model hydrolysis based on pH, with pH specified as a random variable.

MODE: User option for Monte Carlo simulation. Set Mode=1 to generate K from underlying variables of particle size and gradient, set Mode=2 to estimate K as a log-normal distribution independent of particle size.

XS: X-coordinate of origin of grid, in appropriate units. Range 0. to 5000.

YS: Y-coordinate of origin of grid, in appropriate units. Range 0. to 5000.

DXOB: Grid spacing (interval) in the X direction. PLUM2D thus specifies an evenly spaced grid.

DYOB: Grid spacing in the Y direction, may differ from DXOB and is typically smaller than DXOB.

V: Average Darcy velocity of uniform regional flow, in the appropriate units, coincident with x axis. Required in deterministic mode only. In Monte Carlo mode V will be generated from underlying hydrogeologic variables, using the methods described by Mulkey and Brown (1985).

M: Average aquifer saturated thickness, which is assumed constant.

P: Effective porosity (as a fraction). Required in deterministic mode only.

L: Longitudinal dispersivity, in units of length. Note that this model requires input of dispersivity, rather than dispersion coefficients.

T: Transverse dispersivity, in units of length.

RD: Retardation coefficient. $RD = V/V_c$, where V is the regional velocity and V_c the apparent velocity of the contaminant. Thus RD must be ≥ 1 . Enter RD=1 for no

retardation.

HL: If radioactive decay has been specified, enter half life, in years.

The next eight variables are required only in the Monte Carlo mode:

ITER: Number of iterations (runs) for Monte Carlo mode. ITER is recommended to be set to at least 500 to provide adequate definition of the frequency histogram. However, the user will usually wish to first test model performance by setting ITER to a smaller number.

CVL: Coefficient of variation of leachate (injection) concentrations, where the coefficient of variation is the standard deviation divided by the mean. The injection concentrations are modeled as a normal process.

TH(1), TH(2): The mean particle size is modeled as a log-10 uniform process, measured in centimeters. TH(1) is the maximum of the range of the mean, while TH(2) is the minimum. Thus TH(2) must be \leq TH(1). GR(1), GR(2), GR(3): The hydraulic gradient is modeled as a triangular distribution, in which GR(1) is the most likely value, GR(2) the minimum value and GR(3) the maximum value. The range of GR is restricted to 1.0E-5 to 0.1, expressed as length per length.

CVD: Coefficient of variation for dispersivities, applied to both L and T.

CVLNQ: Coefficient of variation of leaching (injection) rates. If the HELP model has been applied to this site the observed coefficient of variation from the HELP results will be reported.

DKLN: Required only if MODE is set to 2, and hydraulic conductivities are to be independently generated. DKLN is then the mean of the natural log of hydraulic conductivity, in cm/sec.

DKLNV: Standard deviation of mean LN hydraulic conductivity. Required only if MODE is set to 2.

DATA SET 1: OBSERVATION POINTS. Required only in Monte Carlo mode. For each observation point specified by NOBS the user must enter the x and y grid index (IXOBS and IYOBS).

DATA SET 2: INJECTION WELLS. For each injection well, or source modeled as an injection well, the user must enter the following values:

X: x grid coordinate of the source.

Y: y grid coordinate of the source.

Q: injection rate of the source, specified as gpd or m^3/d , as chosen by UNITS.

C: solute concentration of injection, as mg/l or ppm.

TIME: time since start of injection (operation) of this source, in days.

4. DUPVG

The above two analytical models are limited in their use to situations in which the aquifer can be modeled as approximately equivalent to a confined aquifer. Serious problems with this assumption arise when leaching from a source is of sufficient volume relative to regional flow to create a significant radial flow component. The source then serves not only to introduce contamination, but also alters the flow regime, and the aquifer will possess a moving free surface. The significance of such effects is estimated in the CHOICE algorithm by a preliminary calculation of ground water mounding resulting from the source. Where significant movement of the free surface is expected few analytical solutions are available. Model DUPVG provides a solution for a particular class of these problems (Volker and Guvanasen, 1987; Guvanasen and Volker, 1982).

DUPVG is a two-dimensional model in the X-Z plane, considering the longitudinal and vertical distribution of the contaminant. The geometry is thus an extension of the one-dimensional case. The source is represented as an infinitely long recharge basin of a fixed width which contributes a constant rate of recharge to the aquifer. The aquifer is assumed to be symmetrical in X about this source, and bounded by a constant head drain at a fixed distance, and there is assumed to be no pre-existing regional flow pattern. This enables the calculation of an approximate velocity distribution within the saturated zone, and thus contaminant distribution. The assumption of an infinitely long recharge basin implies that this model will be appropriate when the point of observation is sufficiently close to the source so that the effect of finite lateral extent of the source is unimportant, as in the application of ODAST. DUPVG is thus particularly important for estimation of plume development near to a large areal source which contributes significantly to the flow regime, such as surface irrigation systems.

It should be reemphasized that the only flow considered by DUPVG is that induced by the source. Thus dispersion is the only mechanism for dilution of the source concentration. As decay is not considered, this means that if DUPVG is run for a sufficiently long time it will eventually "flood out" the aquifer with water at the source concentration. It is thus not particularly useful to run the model for predictions at a given distance if the time involved is sufficient so that water at source concentration has fully occupied this point - for in this case the prediction is merely that the concentration is

equal to the source concentration. A rough estimate of the occurrence of this phenomenon is when:

$$\frac{Q A t}{7.48 s n R} \gg x \quad (23)$$

where Q is the areal leaching rate in gallons per day per square foot, A is the half-width of the source along the direction of flow, in feet, t is time in days, s is the initial saturated thickness, in feet, n is porosity, R is retardation coefficient (v/v_c) and x is distance to the observation point in feet. Where this inequality holds the controlling criteria for concentration predictions will be the determination of Q, and any vadose zone attenuation of contaminant load. The analyst may also need to consider whether any processes of decay or dilution by regional flow, which cannot be considered by this model, may have a significant effect.

In order to derive the analytical solution a number of important simplifying assumptions were made, and the user should be aware of the implications of these assumptions. The solution method first assumes that the rise of the free surface is substantially less than the initial saturated thickness of the aquifer (tests of this condition are made in the CHOICE algorithm). Based on this premise it is assumed that:

(1) The unsteady free surface can be approximately described by a streamline, which implies that the flow pattern is equivalent to the confined case, but with an a priori unknown upper boundary.

(2) Near the source, streamline and equipotential functions change little with time, so that the transient velocity can be described by a steady state distribution modified by a simple time function.

(3) Further away from the source the velocity field is essentially horizontal and its spatial variation is negligible.

These conditions require that the slope of the free surface is relatively small, and that the distance to the constant head drain is sufficiently large so that equipotential lines at the downstream end are vertical. The final solution uses an approximation that is equivalent to the case where the distance to constant head goes to infinity, although the near source velocities are first computed using a finite value of this distance. In any case, the solution method will be accurate only when the constant head boundary is relatively far away from the source. Further, constant head boundaries must be assumed to be distributed symmetrically about the source axis.

The approximate solution employed for the transport equation is based on the assumption that the distance to constant head can be extended to infinity. However, the velocity distribution is first calculated without this approximation. Thus the solution

method should provide an accurate estimation of the average position of the front. However, when the constant head boundary is closer to the source the vertical distribution of concentrations may not be accurate.

Other important limitations are obvious from the nature of the solution. The method cannot take into account any regional flow other than that induced by the source. Further, the method treats only conservative substances, which may be retarded but are not subject to decay.

The preprocessor for DUPVG uses an interactive mode, the user types in the free-format input data interactively through the main screen. The input data are as follows:

NUMX: Number of points modeled in the X direction, which establishes the 1-dimensional grid. From 1-25 points may be used. Grid size does not affect solution, and for Monte Carlo simulation you will normally wish to examine only one or two points at the perimeter of compliance to speed execution.

NUMZ: Number of points modeled in the vertical, Z direction, counting downward from the top of the saturated zone.

NUMT: Number of time steps for calculation.

Q: leaching rate from source expressed as gal./ft² - d. If the HELP model has been run for this site, the values obtained will be reported here. In DUPVG the source is conceived as a basin of infinite horizontal extent and finite width.

POR: Total porosity of the medium.

B: Thickness of saturated layer (initial thickness). This is used to calculate the initial mixed concentration beneath the source.

DL: Longitudinal dispersion coefficient in M²/day.

DT: Transverse dispersion coefficient in M²/day.

A: For DUPVG, this measures the effective width of the "infinite" source along the X (flow) axis. This is properly the distance from the edge of the source to a flow divide. As the geometry is assumed symmetrical this is equivalent to half of the width of the source in X.

R: retardation coefficient, $= v / v_c$, where v is the velocity of the regional flow and v_c the apparent velocity of the contaminant.

C₀: Mean initial source strength, as ppm.

FC: Field capacity (fraction). Porosity = $P_e + FC$, where P_e is the effective porosity.

PKW: In DUPVG, non-Monte Carlo mode, an initial estimate of K is required. In Monte Carlo mode K will be generated in the usual way.

AHW: Determination of the slope of the free surface requires specification of distance to a constant head boundary, assumed to be symmetrical about the source. Note that for the approximation method used in the solution accuracy decreases as the observation point becomes nearer to the constant head boundary.

ATTEN: Fraction of the solute remaining after vadose zone attenuation. If the HELP model has been run a conservative estimate of ATTN can be calculated automatically. This calculation assumes that the substance proceeds downward through the unsaturated zone at pulses equal to the saturated hydraulic conductivity of that zone, subject to retardation, and thus provides a very conservative estimate of residence time.

5. EPAGW

The basic model employed here was developed by the EPA for analysis of restrictions on land based disposal, and is documented in U.S.E.P.A. (1986). The EPA approach is to model the transport of a given substance, subject to hydrolysis and retardation, determining a downflow dilution factor which is used to back-calculate an allowable concentration of the substance in a landfill, given a down-flow standard level. To do this, Monte Carlo simulation is undertaken over all the relevant hydrogeological variables, using a national data set, allowing the formation of generalized regulatory standards for allowable concentrations within the landfill. The method is carefully designed to account for the correlation among simulated parameter values. The transport model employed is Sudicky et al.'s (1983) 3-D steady-state solution, using Gaussian quadrature to solve the integral. We have modified this method in a number of ways. First, if we assume that the site characteristics are known, or can be specified by distributions, the method is readily inverted, so that the "dilution" factor is used to predict downstream concentrations from a specified source, using the same Monte Carlo analysis. Secondly, instead of using a national data base for the hydrogeologic parameters, one of several data bases can be selected that reflects the characteristics of a specific region within North Carolina. The selected data base can then be modified in accordance with any available site-specific data. The method thus becomes appropriate for an analysis of contamination risk in a situation in which little is known about the specific hydrogeology of a site. The objective is then to simulate the expected risk over the range of hydrogeological conditions that are expected to apply for the specific region in which the site is located.

The source in the EPAGW model is assumed to be distributed as a Gaussian

source. The source is thus areal, but concentrated towards a central point. This makes the model particularly applicable to landfills. However, it may be inappropriate for large scale areal sources, such as surface irrigation of wastes, in which contaminant input is relatively uniform across the source area.

EPAGW represents a complete and coherent Monte Carlo approach to contaminant risk analysis under uncertainty. It is thus the model of choice for preliminary analysis of risk in situations in which little site specific data is available on flow regime and hydrogeology, given that a Gaussian representation of source distribution is appropriate. The model development assumes that the direction of flow from the source is not accurately known. Analysis is thus made at a specified distance along the (unknown) main axis of flow. Equivalently the model may be applied to analysis along an explicitly known axis of flow.

EPAGW contains detailed routines for calculation of chemistry dependent hydrolysis of contaminants. It also considers the effects of vertical mixing. The model will thus also be useful for analysis in some situations where there is substantial knowledge regarding the flow regime, but the analysis requires consideration of partial penetration and/or complex hydrolysis reactions. This is especially useful for analysis of certain organic constituents with pH dependent hydrolysis rates.

EPAGW provides a highly flexible method for analysis. However, it can only be applied in the Monte Carlo mode. Further, solution is provided only at a point along the axis of flow at the surface of the aquifer. A steady-state concentration only is calculated, so that EPAGW cannot be used to calculate time history of contamination. From the nature of the solution the model will not be appropriate for large uniform areal sources, such as land applications. The usual assumptions of steady-state, uniform flow apply here, and the model will not be appropriate for sources that contribute a volume of fluid sufficient to significantly alter the flow regime.

Data input for EPAGW consists of two phases. The first phase concerns the parameters controlling site hydrogeology. To initiate this phase for a new site the user should first load a default regional data set from the list provided. Even where an appropriate regional data set is not available one should be loaded to guide input, then modified as needed.

Development of regional data sets is still in progress, but limited by available information. For regulatory analysis it will most commonly be the surficial aquifer that is of interest. These can be conveniently grouped according to the nature of the surface soil. The specification of the underlying hydrogeologic parameter distributions and their probability parameters is designed to allow a maximum of flexibility in selection. First, a regional data base with assumed distributions and metaparameters is selected. Where no additional site data or user knowledge is available, simulation may proceed with these unaltered distributions and values. This will provide an estimate of contamination risk

based on the average characteristics of the area, and so should be modified to reflect any known differences of a specific site location from the average characteristics of the area. However, any parameter distribution may be altered in one or more of the following ways:

1. Respecify parameter distribution metaparameters.
2. Automatically update regional data by combination with site data.
3. Respecify parameter distribution type.

Where the user feels that a given parameter is known with considerable accuracy this may be indicated by specifying the distribution as a tightly restricted uniform or triangular distribution.

The types of distributions that may be specified for the various parameters are identified as follows:

0. No distribution has yet been specified. This must be replaced before running the model.

1. Triangular distribution. The user must specify most likely, minimum and maximum values for the distribution. The triangular distribution is an ad hoc, empirical distribution which takes a triangular shape. This can be used to readily approximate various peaked but skewed distributions.

2. Uniform distribution. The user must specify the minimum and maximum of the range.

3. Log10 Uniform distribution, in which the log values are uniformly distributed. The user must specify the UNTRANSFORMED minimum and maximum values of the range.

4. Normal distribution. The user must specify the mean and standard deviation.

5. Log-normal distribution, in which the log values are normally distributed. The user must specify the mean and standard deviation of the log transformed values.

6. Exponential distribution, in which the mean is equal to the standard deviation. The user must specify this single value.

7. Table-specified distribution. This is available in certain cases only.

Each of the pre-specified regional data sets will describe each of the parameter distributions by one of the above distributions. However, these may vary from data set to data set. For this phase of input, distributions must be specified on the following parameters:

DIAM: mean particle diameter (cm). Note that the specification is of the distribution of the mean, not the full range of particle diameters encountered.

GRAD: gradient of the water table (length per length).

FOC: organic carbon fraction of aquifer medium. This is an important factor in the chemical analysis of the fate of certain organic constituents.

PH: pH of groundwater.

T: groundwater temperature (Centigrade).

TH: thickness of the saturated zone (meters).

H: leachate initial penetration depth into the saturated zone (meters). This specifies vertical mixing beneath the site. Because of constraints in the solution method H must be equal to at least 2 meters.

QC: leaching rate distribution for engineered (lined) facilities.

QD: leaching rate distribution for non-engineered facilities (Default is table specified; for direct input use m/yr). If the HELP model has been applied to the site the leaching rates estimated from this model may be loaded to replace both the QC and QD values.

Phase one thus requires specification of the general characteristics of the aquifer. Phase two of data input requires information on the site engineering and the contaminant of interest. The following data is required:

CLM: mean leachate concentration, in mg/l (ppm).

CLS: standard deviation of leachate concentration mean.

DKAO: hydrolysis rate for the substance under acid conditions, 1/[molar*year]. EPAGW simulates the lumped degradation constant, K, based on pH, DKAO, DKB0 and DKN0, using equation 2. These values must be converted to year⁻¹ for input into EPAGW.

DKB0: base catalyzed hydrolysis rate, 1/[molar*year].

DKN0: neutral catalyzed hydrolysis rate, 1/year.

DKOW: log₁₀ octanol/water partition coefficient for contaminant, describing the constituent's solubility. The actual value will be dependent on the organic carbon content and available surface area of the soil. If this value is not directly known it may be estimated from:

$$DKOW = 5.0 - 9.67 \log_{10} (SW) \quad (24)$$

where S_w =solubility in water. EPAGW also uses DKOW to estimate the adsorption coefficient of the constituent, using the approximate relationship:

$$\log_{10} K_{oc} = 1.029 \log_{10} K_{ow} - 0.18 \quad (24)$$

Note that this relationship may not be valid for polar constituents.

ATTN: a factor which specifies the fraction of solute remaining after passage through the unsaturated zone beneath the landfill. If the HELP model has been applied to this site a conservative value of ATTN may be calculated automatically from the HELP output. This is calculated in the same manner as for the model ODAST.

NPROB: number of Monte Carlo runs. A minimum of 500 is recommended for adequate definition of the cumulative frequency. However, the user will usually wish to test model performance by first trying a smaller number of runs. The value of NPROB is not saved with the data set, but defaults to 500, and thus may need to be respecified for each run.

AW: surface area of landfill, in square meters.

TR: reference temperature for the chemical rate constants, in degrees C (these are usually specified at 25° C).

XX: distance from the edge of the disposal area to the observation point, along the flow axis (meters). The exact value of XX is somewhat ambiguous for large areal sites.

Leaching Rate Distribution: Calculated from HELP model, or from table, where
C: table for engineered facilities.
D: table for non-engineered landfills.

6. EPASF

The EPA surface water model (EPASF) was designed to assess impacts of waste disposal sites on surface waters (with hazard associated with human use of contaminated surface waters or consumption of fish from contaminated surface waters) in a manner analogous to the EPAGW model. Here, however, at least two stages must be considered: transport from the landfill via groundwater, and entry into and dilution in the stream. As with the EPAGW model, we have modified this model to provide risk assessment from a given landfill, and have likewise added a preprocessor. EPASF and EPAGW can share essentially the same input data set, with a few additions.

EPASF estimates groundwater contaminant transport to the stream using either a one dimensional or a three dimensional solution, and with or without consideration of dispersion. In the three dimensional case the transport solution is the same as that used in EPAGW. Note that lateral dispersion of the contaminant plume affects the concentration, but not the total mass loading to the stream. As EPASF provides only a very generalized approximation of the transport process analysis without dispersion will often be adequate for a first estimate.

EPASF provides only a rough and preliminary estimate of impacts in surface waters. However, modelling the interaction of groundwater and surface water often presents formidable difficulties, so that one is forced, by default, to rely on a model such as EPASF for a preliminary estimate of risk. It should be remembered however that EPASF presents only a preliminary estimate. If contamination problems are suggested by application of EPASF the user may then need to attempt more sophisticated analysis.

EPASF uses essentially the same data input format as EPAGW, and can share the same data sets. However, distributions for two additional parameters must be specified when characterizing the hydrogeology. These are:

FOCS: organic carbon fraction of suspended sediment in the stream.

FL: lipid fraction of fish biomass. This is needed only when using Scenario 3, in which human impact is assessed via consumption of fish from the stream. The lipid fraction is used to assess bioconcentration of certain lipophilic organic constituents.

Input of the site parameters is very similar to that for EPAGW, but possesses a few differences, including slight alterations in variable names. The site data input for EPASF are defined as follows

DIMNSN: Dimension of problem; the groundwater transport phase may be run using a one dimensional or three dimensional solution. The one dimensional solution of course results in much quicker execution of the model.

DSPRSN: Effects of dispersion may be included (1) or omitted (0).

X: distance from landfill edge to the stream, in meters.

CLM: leachate concentration, mg/L (ppm).

CLS: standard deviation of leachate concentration.

LKOW: log octanol/water partition coefficient for contaminant species.

KHAN: acid catalyzed hydrolysis rate, 1/[molar*year].

KHB0: base catalyzed hydrolysis rate, 1/[molar*year].

KHN0: neutral pathway hydrolysis rate, 1/year.

TREE: reference temperature for hydrolysis rates, degrees C (usually given at 25° C).

NUMRNS: number of Monte Carlo runs. At least 500 runs are recommended, and in most cases this model is moderately fast.

AW: area of waste site, square meters.

AS: area of watershed above point of impact, in square miles. This factor is used in the determination of in-stream dilution.

Leachate distribution: flux of leachate from landfill, in m/yr.

Choices: subtitle C (engineered), subtitle D (nonengineered). As in EPAGW these values may be replaced by rates calculated by the HELP model.

ATTN: factor specifies the fraction of solute remaining after passage through the unsaturated zone beneath the landfill. If the HELP model has been applied to this site, a conservative value of ATTN may be calculated automatically from the HELP output.

7. LTIRD

LTIRD calculates the concentration of a particular solute in radial flow (Javandel et al., 1984), using a semianalytical solution originally written by Moench and Ogata (1981). This model is included for the explicit purpose of treating purely radial flow situations, in which regional flow is not present. The idealized situation treated by the model considers a confined aquifer of constant thickness which is recharged through a fully penetrating well at a constant rate. The model considers steady-state plane radial flow only.

As with other solutions for confined aquifers, LTIRD is applicable as an approximation to unconfined aquifers in cases where mounding is sufficiently small so that the streamlines remain approximately parallel. LTIRD can also be used to treat surface inputs if the assumption can be made that the solute is vertically mixed in the aquifer soon after introduction.

LTIRD has a rather **limited range** of applications in the advisory system. There is no consideration of regional flow, so this model should be used only when the radial flow from recharge dominates, but, in the case of a surficial unconfined aquifer, the rate of

recharge is also sufficiently small so that the assumption of a confined aquifer is approximately valid. Use of the model is also limited by the fact that it does not include decay or retardation, and the fact that it assumes steady-state plane radial flow. The source is modeled as a well, so that the model is not appropriate to areal sources.

Data input for LTIRD is quite simple. The following are required, in any consistent units:

NUMR: Number of radiuses at which to calculate concentrations.

NUMT: Number of time steps to calculate.

RDW: Radius of the well, or source approximated as a well.

R (1 to NUMR): Radial distances at which calculations are made.

T (1 to NUMT): Times for calculation.

ALPHA: Dispersivity.

Q: rate of recharge.

B: Saturated thickness of aquifer.

N: Porosity of aquifer.

C0: Concentration of solute in recharge.

8. RESSQ

RESSQ is a program for semianalytical calculation of contaminant transport (Javandel et al., 1985). The model calculates two-dimensional transport by advection and adsorption (no dispersion or diffusion) in a homogeneous, isotropic confined aquifer of uniform thickness when regional flow, sources, and sinks create a steady state flow field. Recharge wells and ponds act as sources and pumping wells act as sinks. The solution proceeds by calculating the streamline pattern in the aquifer and the location of contaminant fronts around sources at various times. RESSQ can thus be applied to a large variety of complex flow situations that can not be handled by analytical solutions.

Because the method is limited by neglecting dispersion, RESSQ, as other semianalytical methods, is most appropriate for preliminary analysis of the extent of probable contamination in a complex flow regime. If the semianalytical method does suggest a contamination problem at the perimeter of compliance the user may then need

to apply a more complex numerical model. Because it is a preliminary analysis tool, RESSQ is provided only in a deterministic mode.

The most obvious **limitations** of RESSQ are its neglect of dispersion and decay. Other limitations of the method are similar to those that apply to most two dimensional steady state analytical solutions. RESSQ requires that the medium is homogeneous and isotropic, with steady state uniform regional flow. Thus the method is not applicable when the medium is distinctly heterogeneous or anisotropic. Further, the method is not directly applicable to transient problems.

A more subtle limitation is due to the assumption made in the model that a steady state flow field exists. This implies that the sum of flow rates from all the injection wells should be equal to the sum of the flow rates from all the production wells. In practice, RESSQ can be applied to situations where these sums are not equal, if analysis is made at sufficiently large values of time so that quasi-steady flow prevails (see below). However, if attempts are made to apply the model to shorter time periods where the two sums are widely different bizarre results may occur. Note that this problem is avoided if a constant head boundary is specified through the use of image wells, in which case the two sums will be by definition equal.

The solution method used in the model is based on the assumptions of a uniform, confined aquifer. Application to a surficial aquifer is thus valid only when conditions in the surficial aquifer approximate those of a confined aquifer. For a preliminary analysis of contaminant risk this is appropriate when the surficial aquifer does not show distinct seasonal variability, and the input from sources does not result in substantial mounding. The latter condition should be adequately met in situations for which the Dupuit approximations hold. In addition, and like most available two-dimensional analytical solutions, RESSQ assumes that sources fully penetrate the aquifer. This is equivalent to assuming that the contaminant loading from a source instantaneously displaces the preexisting water throughout a vertical column of the aquifer. Note that RESSQ provides a sharp front approximation, and cannot account for mixing of the flow from a source with the water in the aquifer. Instead, the source flow displaces the water in the aquifer, without mixing. For a source that is not actually fully penetrating this approximation is obviously more valid for a thin saturated layer. However, an overly thin saturated layer is likely to result in violation of the confined aquifer approximation. The practical result is that RESSQ, when applied to a surficial aquifer with a nonpenetrating source, is likely to provide inappropriate concentration results in the region close to the source, but more accurate results further away from the source.

Attempts to apply RESSQ to surficial sources which do not fully penetrate the aquifer are considerably complicated by the necessary assumption that no mixing occurs. This may result in overestimation of the concentration resulting from a source. This is a particular problem when the rate of regional flow is significantly large in relation to the rate of recharge from the source. In such cases the positions of contaminant fronts

can still be calculated, but the concentration within these fronts cannot be interpreted as equal to the source concentration. In general, RESSQ is recommended for approximate application to surficial sources only in cases where the flow from such sources is of sufficient volume to overwhelm the regional flow in the neighborhood of the source and a radial flow pattern is established. In sum, it should be emphasized that RESSQ is best thought of as a preliminary analysis tool. Despite the many limitations expressed above it provides a very powerful tool for preliminary analysis of complex flow situations.

Appropriate use of RESSQ is somewhat of an art, and will require practice on the part of the user to obtain adequate results. This is because the model calculates concentration front positions on the basis of a finite number of streamlines. The results observed are thus to a degree sensitive to the number of streamlines modeled, and the starting angle of the first streamline leaving each source. The user may need to experiment with these values to obtain the desired results.

By proper formulation of the input data RESSQ can be used to model a wide variety of situations. The following suggestions for data input are taken from Javandel et al. (1984):

(1) If the total flow rate from all injection wells does not equal the total flow rate from all production wells, then, strictly speaking, a steady state flow field, as required by RESSQ, cannot be achieved. However, for large values of time one may assume that quasi-steady flow prevails, thus allowing RESSQ to be used. However, if the sum of the two rates are widely divergent, unexpected and inappropriate results may be found for shorter time periods.

(2) In addition to modeling recharge or injection wells as point sources, RESSQ can model constant head ponds as finite radius sources. This is done by specifying the pond as a recharge well, with radius of the pond specified as the radius of the well. Such sources are however also considered to be fully penetrating.

(3) RESSQ can include a linear no-flow or constant potential boundary using the method of images. A boundary is represented by adding an image well for each real well in the problem, with the boundary located on the perpendicular bisector of the line connecting each real well/image well pair. For a no-flow boundary the real and image wells have the same flow rate, that is, either both are injection or both are production wells. Since there is no flow through an impervious boundary, the only regional flow allowed in this case is parallel to the boundary. For a constant potential boundary the real well/image well pairs have flow rates equal in magnitude and opposite in sign. In this case the boundary must be an equipotential and the only regional flow allowed is perpendicular to the boundary.

(4) The model requires that the number of injection wells specified must be greater than zero. This is because injection wells act as the starting points for streamlines, so

without injection wells no streamline pattern can be draw. To allow greater flexibility in presenting streamline patterns. Zero-flow wells do not affect the velocity field, but provide starting points for streamlines whose paths may help explicate the velocity field created by regional flow and nonzero-flow rate sources and sinks present.

(5) The techniques described in (4) allow the specification of a uniform regional flow by use of a row of zero-flow-rate wells. Streamlines describing regional flow can be drawn by placing a row of zero-flow rate wells perpendicular to the direction of regional flow at a distance relatively far from sources and sinks. The spacing between these wells must be determined as a function of the ratio of source flow rate to regional flow Darcy velocity. A routine (ZQWELL) is incorporated into the model preprocessor to provide for automatic calculation of the required line of zero-flow wells to describe the regional flow. However, the user may find it necessary to experiment with the input for this routine in order to establish a sufficiently small (or sufficiently large) number of such wells to describe the regional flow within the data input limitations of the code.

RESSQ, by neglecting dispersion, provides a sharp-front approximation of contaminant concentration. That is, water injected from a source undergoes no mixing with water already present in the aquifer, but displaces that water without dilution. Output of RESSQ includes plots of the time position of contaminant fronts around sources. Because these represent sharp fronts, the predicted concentration within the fronts is equal to the injection concentration, while the predicted concentration outside the fronts is equal to the ambient aquifer concentration. In actuality, the processes of dispersion and dilution should result in contamination extending beyond the position of the predicted fronts, but with a corresponding dilution of concentration. The user should pay careful attention to this phenomenon in interpreting the results.

If a production well is specified, the time evolution of concentration at the production well will be estimated (provided that at least two stream lines reach the production well during the simulation period). This time evolution is based solely on the number of streamlines from sources captured by the production well, and does not consider the effects of dispersion and dilution.

Input data for RESSQ requires the following information:

NWI: Number of injection wells (> 0), not including zero flow wells automatically specified in routine ZQWELL.

NWP: Number of production wells. May be zero, but see cautions regarding application of the model to non-steady state flow patterns.

CO: Ambient (preexisting) contaminant concentration in the aquifer.

CD: Default concentration of injection wells. This number can be overridden in the

specifications for each well (below). However, it is necessary to specify C0 if the user wishes to observe the dimensionless concentration evolution at production wells. In general, the user should specify C0 equal to the highest injection well concentration.

UNITC: Units of concentration. This is a character string used to label output. The default value is "Percent"

IZO: Requests the use routine ZQWELL for automatic calculation of a line of zero flow wells to specify uniform flow (1: yes, 0: no). Generally the user will wish to enter 1 if regional flow is present.

ATTEN: (Default = 1.0). This option is provided for use with surficial sources. In such cases the strength of the contaminant may decrease significantly in the process of percolation through the unsaturated zone. The users may thus specify ATTEN to represent the fraction of the actual source concentration remaining when the flow from the source enters the aquifer.

HEIGHT: Average saturated thickness of aquifer (in feet). This value is assumed to be constant throughout the region of study.

POR: Effective Porosity of the aquifer, expressed as percent ($POR = P \times 100$).

V0: Pore water velocity of uniform flow (ft/day).

ALPHA: Direction of regional flow, in degrees, measured counter-clockwise from the positive X axis.

ADSORB: Adsorption capacity of matrix, equals $(1-1/R)$, where R is the retardation coefficient. The range of ADSORB is 0-1, as $R = V/V_c$, where V is the regional velocity and V_c the apparent velocity of the contaminant.

NFRNTS: Number of contaminant front positions to be calculated for each source (maximum 7).

DATE(1 to NFRNTS): Times at which fronts are to be calculated (in years).

TMAX: Period of study in years. This sets the maximum amount of time for calculating the trace of streamlines, and thus should be substantially greater than the time period of interest. TMAX should be set large enough so that streamlines can be fully drawn throughout the area mapped. The example problems given by Javandel et al. (1984) use $TMAX=200$, if you are specifying regional flow through use of zero-flow wells, TMAX should be long enough so that these flow lines can be drawn across the area to be mapped.

DL: The step-length or spatial increment used to trace out the streamlines, in feet. If left blank this defaults to $(XMAX-XMIN)/200$. Using a larger step-length will decrease run time, but will also decrease the resolution of the streamline plot.

NTL: Plot option, set $NTL = -1$ to suppress plot of streamlines.

NTF: Plot option, set $NTF = -1$ to suppress plot of pollutant fronts.

XMIN: Origin of area of study, X axis (in feet). It is often convenient, particularly when specifying regional flow, to set up the axes so that $\{X=0, Y=0\}$ is the center of the area of study.

XMAX: Limit of area of study, X axis (in feet).

YMIN: Origin of area of study, Y axis (in feet).

YMAX: Limit of area of study, Y axis (in feet).

The next seven variables control the automatic calculation of a row of zero-flow wells to simulate uniform regional flow. They will be requested only when $IZQ=1$. The number of ZQWELLS calculated will be displayed after the data is input. If this number is too large you may modify the input and try again. In this case instructions for modification will be displayed.

XREF: X coordinate of arbitrary reference point near the sources and sinks (in feet).

YREF: Y coordinate of the arbitrary reference point.

DIST: Distance from reference point to row of zero flow wells, in feet. Ideally, DIST must be large enough so that near the zero-flow rate wells the streamlines are essentially parallel.

WIDTH: Width of the row of zero-flow wells (in feet). This determines the area that will be covered by the regional flow streamlines

Q1: Flow rate of the first source (injection well) in gpd. This value will be carried to the source input screen as well.

NSL1: Number of streamlines calculated for the first source.

ITR1: Ratio of NSL1 to the number of streamlines plotted for the first source.

WELLS: The following data must be specified for each source and sink (injection well and source well). The injection wells (sources) must be specified first. Monitor source wells may be specified in order to observe contaminant concentration development.

NAMEW: Name of the well, source or sink (character).

XW: X coordinate of the well (feet).

YW: Y coordinate of the well.

QW: absolute value of flow from/to this well, gpd.

RADDW: radius of well (or pond), in feet. This value will default to 0.2461 ft.

C: concentration of an injecting well in units of UNITC. This will default to C_0 .

BETA1: angle (degrees) of the first streamline calculated for each injection well. This value can be modified to obtain better streamline definition. The angle is calculated counter-clockwise from the positive X axis.

NSL: number of streamlines calculated for an injection well. Default value is 40. Set NSL = -1 for no streamlines.

ITR: ratio of NSL to number of streamlines actually plotted. Determines the density of the plot. Set ITR = -1 to suppress plotting of streamlines from this well.

INDW: Plot option. Set INDW = -1 to suppress plot of fronts in the case of an injection well, or suppress study of concentration in the case of a production well.

The graphical output from this UNIX version is the same as that from DOS version (see Figure 30 in Section III).

9. USGS MOC

The Method of Characteristics (MOC) model developed by Konikow and Bredehoeft (1978) is a well-tested and accepted, highly flexible two-dimensional numerical groundwater transport model. Unlike analytical models, this model considers heterogeneity and anisotropy of the porous medium, and offers great flexibility in specifying sources, sinks and boundary conditions. The version included in the Advisory System includes several updates distributed since the publication of the 1979 manual

that extend the method to allow consideration of retardation and radioactive-like decay in the model.

By using a numerical method, the characterization of the aquifer is not constrained by the availability of analytical solutions. The numerical method requires that the area of interest be subdivided by a grid into a number of smaller subareas. MOC utilizes a rectangular, uniformly spaced, block-centered, finite-difference grid, in which nodes are defined at the centers of the rectangular cells. If sufficient information is available, the user may individually specify distinct values of controlling parameters at each of these nodes. The technique employed seeks numerical solutions first to the head distribution, then to the flow equation, and finally to the transport equation. The transport equation is solved using the Method of Characteristics, which avoids the problem of numerical dispersion often encountered in numerical models.

The UNIX version of the Advisory System uses a modified MOC for use in Monte Carlo simulation. However, only some of the many possible sources of uncertainty are considered in this procedure. These were selected on the basis of a sensitivity analysis, under the assumption that the hydraulic heads along the boundaries are exactly known. Thus the Monte Carlo method is not implemented in full generality here, but rather designed to be most applicable for the specific case of analysis of proposed hazardous waste landfills. Of particular interest in this method is the specification of a spatially covariant hydraulic conductivity random field, which is well adapted to the simulation of the natural uncertainty in this parameter, where it is expected that hydraulic conductivity values will tend to show a higher degree of similarity between nodes that are closer together in space. The Monte Carlo procedure can handle the situation in which contaminant input begins following the failure of a containment structure. This scenario applies to the analysis of a proposed hazardous waste landfill, in which the analyst must consider the possibility of contamination resulting from failure of the landfill liner.

It is well documented that the spatial variability of hydraulic conductivity can have a significant effect on the field-length dispersion of contaminant plumes and that hydraulic conductivity is lognormally distributed (Freeze, 1975; Smith and Schwartz, 1980, 1981). We assume a two level stochastic model to reflect both natural and parameter uncertainty in the hydraulic conductivity field distribution. In this UNIX version Advisory system, three steps are developed to obtain up to 100,000 simulations of hydraulic conductivity random field. In the Advisory System, there are three steps in constructing the random field of hydraulic conductivity:

a. Input prior information

This step requests prior information of hydraulic conductivity, and observation (field) data. The prior information includes mean value, variance and correlation length for hydraulic conductivity. This procedure has been written in FORTRAN code named 'premain.f'

b. Bayesian update of hydraulic conductivity

Having the prior information and observation data, the probability characteristics of hydraulic conductivity random field can be updated using Bayesian update technic. This technic has been proposed by Kitanidis(1990) and applied by Liu(1993). The solving algorithm has been written in a FORTRAN code named 'mainn.f'.

c. Realization of hydraulic conductivity random field

Having the spatial probabilistic distribution of hydraulic conductivity, the realization of hydraulic conductivity random field is accomplished by using Monte Carlo simulation program, COV. COV uses a matrix decomposition scheme as a mechanism for generating two-dimensional fields of a normally or log-normally distributed parameter(i.e. hydraulic conductivity). The input data for the program consists of a set of X, Y-coordinate locations and parameters which represent the distribution of the parameter of interest. The generating scheme is as follows: the program computes the covariance matrix for a set of different locations and decomposes this matrix into a lower-triangular matrix. The decomposed matrix is then used to estimate a set of values for the parameter of interest. These values may be either normally or log-normally distributed. A seed which changes automatically is incorporated into the program to generate different realizations of the parameter field.

MOC, particularly in the deterministic mode, provides a highly flexible tool for analysis of many contaminant transport situations. However, the user must also be aware of certain **limitations**. The development of the solution required a number of assumptions, and the degree to which field conditions deviate from these assumptions will affect the applicability and reliability of the model. These include the following:

- (1) Darcy's law is valid and hydraulic-head gradients are the only significant driving mechanism for fluid flow. Low velocity flow under other conditions is not considered.
- (2) Solute transport is dominated by convective transport, an assumption required for the method of characteristics solution of the flow equation.
- (3) The porosity and hydraulic conductivity of the aquifer are constant with time, and porosity is uniform in space.
- (4) Gradients of fluid density, viscosity, and temperature do not affect the velocity distribution.
- (5) No chemical reactions occur that affect the fluid properties or the aquifer properties.
- (6) The only chemical reactions considered for the solute species are linear

retardation of velocity and decay that can be described as similar to radioactive decay. No pH dependent hydrolysis of constituents is considered.

(7) Ionic and molecular diffusion are negligible contributors to the total dispersive flux.

(8) Vertical variations in head and concentration are negligible.

(9) The aquifer is homogeneous and isotropic with respect to the coefficients of longitudinal and transverse dispersivity.

The model in general is applicable to both confined and unconfined aquifers. However, the validity of the present code is somewhat limited in application to unconfined aquifers. That is, the saturated thickness is presently specified independent of the water-table elevation, and does not change in response to changes in water-table elevation. This means that if recharge and/or pumping do result in substantial changes in water-table elevation the solution will lose accuracy in the unconfined situation. The user should be particularly careful in attempting to apply the model to transient flow problems in an unconfined aquifer.

Additional limitations apply to the use of this model in the Monte Carlo mode. The most important practical limitation is that run time may be very long when using this model on a Workstation. As noted above, the Monte Carlo formulation used here considers only certain specific sources of variability. If there are other sources of variability that have an important affect on predicted concentrations use of the Monte Carlo method provided here will not provide an accurate analysis of risk.

Finally, in both the deterministic and the Monte Carlo mode, the user must specify the head in the aquifer at the start of the simulation, as an initial condition. Obviously, in many cases complete data on head distribution will not be available; however, no provisions have been made to account for uncertainty in initial heads. It is possible to determine initial heads from previous simulations. However, it is important to note that the simulation results may be sensitive to variations or errors in the initial conditions. In discussing computed heads, Trescott, Pinder and Larson (1976) state: "If initial conditions are specified so that transient flow is occurring in the system at the start of the simulation, it should be recognized that water levels will change during the simulation, not only in response to the new pumping stress, but also due to the initial conditions. This may or may not be the intent of the user."

MOC is provided with a DOS version preprocessor for data input supplied by the International Ground Water Modeling Center and written by P. Srinivasan. We have used the format of this preprocessor as a model for the development of the UNIX version preprocessor in the system. The preprocessor supplied by IGWMC has been modified by us to allow input of the additional data required for Monte Carlo simulation.

Considerable flexibility is available in the model through the specification of boundary conditions. Two general types are incorporated into the model, being constant-flux and constant-head boundaries. These can be used to represent the real boundaries of an aquifer as well as to represent artificial boundaries for the model which can be used to minimize the areal extent of the modeled part of the aquifer. The following descriptions of boundary conditions are taken directly from Konikow and Bredehoeft (1978).

A constant-flux boundary can be used to represent aquifer underflow, well withdrawals, or well injection. A finite flux is designated by specifying the flux rate as a well discharge or injection rate for the appropriate nodes. A no-flow boundary is a special case of a constant-flux boundary. The numerical procedure used in the model requires that the area of interest be surrounded by a no-flow boundary. Thus the model will automatically specify the outer rows and columns of the finite-difference grid as no-flow boundaries. No-flow boundaries can also be located elsewhere in the grid to simulate natural limits or barriers to ground-water flow. No-flow boundaries are designated by setting the transmissivity equal to zero at appropriate nodes, thereby precluding the flow of water or dissolved chemicals across the boundaries of the cell containing that node.

A constant-head boundary in the model can represent parts of the aquifer where the head will not change with time, such as recharge boundaries or areas beyond the influence of hydraulic stresses. In this model constant-head boundaries are simulated by adjusting the leakage term at the appropriate nodes. This is accomplished by setting the leakage coefficient to a sufficiently high value (such as 1.0 s^{-1}) to allow the head in the aquifer at a node to be implicitly computed as a value that is essentially equal to the value of H_0 , which in this case would be specified as the desired constant-head altitude. The resulting rate of leakage into or out of the designated constant-head cell would equal the flux required to maintain the head in the aquifer at the specified constant-head altitude. If a constant-flux or constant-head boundary represents a fluid source, then the chemical concentration in the source fluid must also be specified. If the boundary represents a fluid sink, then the concentration of the produced fluid will equal the concentration in the aquifer at the location of the sink.

The model allows the specification of a time-varying pumping schedule through the specification of a number of pumping periods. During each of these periods the pumping occurs at a constant rate. However, differing pumping configurations may be specified for subsequent pumping periods. For Monte Carlo simulation the model should be run in steady-state mode with only one pumping period specified.

The input data is organized by "card images," as follows:

- card 1. Title
- card 1a. Monte Carlo card I
- card 1b. Monte Carlo card II
- card 2. Control card I
- card 2a. Control card Ia (optional)
- card 3. Control card II
- card 3a. Control card IIa (optional)
- data set 1. Observation points.
- data set 2. Wells
- data set 3. Transmissivity.
- data set 4. Aquifer thickness
- data set 5. Recharge/discharge.
- data set 6. Node identification matrix.
- data set 7. Instruction for node id's .
- data set 8. Initial head.
- data set 9. Initial concentration . . .
- data set 10. Additional pumping periods.

The two Monte Carlo control cards are, of course, required only when the model is used in Monte Carlo mode.

When the preprocessor for MOC is accessed and the site has not been previously analyzed using this model a default data set may be loaded to guide data input. If previous analysis has occurred the previously formulated data set will be reloaded.

Details for the input "cards" follow:

CARD 1. TITLE

TITLE: Title of the problem and contaminant studied (to 80 characters).

MONTE CARLO CARD 1. This card gives a warning for the selection of Monte Carlo simulations:

"Warning: It will take hours or even days to complete the Monte Carlo routine depending on how many number of simulations you choose!"

MONTE CARLO CARD II. Yes/no option for the selection of using Monte Carlo simulations.

CARD 2. CONTROL CARD I.

NTIM: Maximum number of time steps in a pumping period (limit 100).

NPMP: Number of pumping periods to be specified.

NX: Grid set-up, number of nodes in x-direction.

NY: Number of nodes in y-direction.

NPMAX: Maximum number of particles traced (limit 6400).

NPNT: Number of time steps between printouts. In the Monte Carlo mode a printout will be made after the first run. Subsequent printouts can be suppressed by specifying NPNT > NTIM.

NITP: Number of iteration parameters (usually between 4 and 7).

NUMOBS: Number of observation points to be specified in a following data set (maximum 5).

ITMAX: Maximum number of iterations to be used in the ADI (alternating direction implicit) solution procedure of the flow equation (usually between 100 and 200). A warning will be issued if this value is exceeded without convergence. The authors note that it may be difficult to obtain a solution using the iterative ADI procedure for cases of steady-state flow when internal nodes of the grid have zero transmissivity and for cases in which the transmissivity is highly anisotropic.

NREC: Number of pumping or injection wells to be specified. One such well is allowed per node.

NPTPND: Initial number of particles per node (allowable values 1,4,5,8,9, or 16). Increasing NPTPND decreases the mass balance error, but also substantially increases required CPU time for execution. The user can examine reported mass balance errors on the output. There will often be a trade-off between NPTPND and CELDIS in determining the accuracy, stability and time requirements of the solution, depending on whether or not CELDIS is the limiting stability criterion. The authors recommend specifying NPTPND as 4 or 5 for initial model calibration, then increasing NPTPND to 9 or 16 for final runs when maximum accuracy is desired. Higher values of NPTPND may not however be practical in Monte Carlo mode, due to length of execution time required.

NCCODES: Number of node identification codes (maximum 10). These codes will be used to specify characteristics of identified nodes in a later data set.

NPNTMV: Particle movement interval (IMOV) for printing chemical data (in Monte Carlo mode enter 0 to suppress printing after the first Monte Carlo run; 99 to print at the end of each run).

NPNTVL: Option for printing computed velocities (0: do not print, 1: print for first time step, 2: print for all time steps).

NPNTD: Option for printing computed dispersion coefficients (0, 1 or 2 - same as for NPNTVL).

NPDELC: Should changes in concentration be printed (1:yes, 0:no).

NPNCHV: Option to write velocity data on unit 7 (0, 1 or 2).

NREACT: Should Retardation and Radioactive Decay be included?

CARD 2a. CONTROL CARD 1a (optional). } This card allows the specification of a subgrid so that solute transport may be specified on a smaller grid than calculation of flow.

MX: X coordinate, within the primary grid, of the UPPER-LEFT node of the transport subgrid.

MY: Y coordinate, within the primary grid, of the UPPER LEFT node of the transport subgrid.

MMX: X coordinate of LOWER-RIGHT node of transport subgrid.

MMY: Y coordinate of LOWER-RIGHT node of transport subgrid.

CARD 3. CONTROL CARD II.

PINT: Pumping period, in years. If more than one pumping period is specified data will be later requested for the subsequent periods.

TOL: Convergence criteria for the ADI iterative solution procedure (usually within 0.01).

POROS: Effective porosity of the medium, assumed constant throughout the aquifer.

BETA: Characteristic length (longitudinal dispersivity) in feet.

S: Storage coefficient (set 0 for steady flow problems).

TIMX: Time increment multiplier for transient flow problems. Ignored if S=0.

TINIT: Size of the initial time in seconds. This is required only for transient flow problems, and is ignored if $S=0$.

XDEL: Width of finite-difference cell in x-direction, in feet.

YDEL: Width of finite-difference cell in y-direction, in feet.

DLTRAT: Ratio of transverse to longitudinal dispersivity.

CELDIS: Maximum cell distance per particle move (between 0 and 1). Increasing CELDIS generally decreases CPU requirements. Effects on mass balance will be problem dependent, but will not affect the solution in problems for which CELDIS is not the limiting stability criterion. Further, if CELDIS is reduced to too small a level oscillations may be found in the initial time period of the solution, particularly if the initial distance that a particle can move is less than the spacing between particles (determined by NPTPND). The authors recommend setting CELDIS to 0.75 or 1.0 for initial calibration, then changing CELDIS to 0.50 for final runs.

ANFCTR: Anisotropy factor, ratio of T_{yy} to T_{xx} .

CARD 3a. CONTROL CARD 11a (optional).} Required only when decay or adsorption are included.

DK: distribution coefficient of the solute.

RHOB: bulk density of the solid.

THALF: half-life of the solute (in seconds).

DATA SET 1. OBSERVATION POINTS. This data set specifies the location of observation wells at which detailed output will be provided. In Monte Carlo applications these will be the points at which cumulative concentration frequencies are calculated. For each observation point the user must enter:

IXOBS: grid index in x of the observation point.

IYOBS: grid index in y of the observation point.

DATA SET 2. WELLS.

Specifies pumping and injection wells. For each well, the user must enter:

IX: grid index in x of the well.

IY: grid index in y of the well.

REC: pumping (>0) or injection (<0) rate of the well, in cubic feet/sec.

CNRECH: solute concentration of injected water. Required only for injection wells.

DATA SET 3. TRANSMISSIVITY (deterministic mode only).

DATA SET 4. AQUIFER THICKNESS.

DATA SET 5. RECHARGE/DISCHARGE.

DATA SET 6. NODE IDENTIFICATION MATRIX.

DATA SET 8. INITIAL HEADS.

DATA SET 9. INITIAL CONCENTRATION (deterministic mode only).

For each of these data sets the user will first be queried for the following.

INPUT: The parameter is (0: constant, 1: varies in space).

FCTR: Constant value (or multiplication factor) for the parameter. If INPUT = 1, the user will then be queried for values throughout the grid. Note that the preprocessor allows block assignment of values to areas on the grid. This procedure is described in the on-screen Help available from the preprocessor.

DATA SET 7. INSTRUCTION FOR NODE ID'S.) The NODE ID's identify special input for the appropriately coded nodes. For each of the codes the user is queried for the following:

ICODE: code number for this node ID. Code 2 cannot be used here, as this is reserved for generated releases in Monte Carlo applications.

FCTR1: leakage at the coded node.

FCTR2: concentration at the coded node.

FCTR3: recharge at the coded node.

OVERRD: Set OVERRD = 0 to preserve values of RECH specified in Data Set 5.

DATA SET 10. ADDITIONAL PUMPING PERIODS. If more than one pumping period is specified, the following data must be entered for each additional pumping

period. (See above, Card image 2, for more detailed discussion of these variables).

ICLK: Should data be revised for this period(1:yes, 0:no).

NTIM: Maximum number of time steps in the pumping period (limit 100).

NPNT: Number of time steps between printcuts.

NITP: Number of iteration parameters (usually between 4 and 7).

ITMAX: Number of iterations in ADIP (usually between 100 and 200).

NREC: Number of pumping or injection wells to be specified.

NPNTMV: Particle movement interval (IMOV) for printing chemical data (enter 0 for printing at the end of the simulation).

NPNTVL: Option for printing computed velocities(0: do not print, 1: print for first time step, 2: print for all time steps).

NPNTD: Option for printing computed dispersion coefficients (0, 1 or 2 - same as above)

NPDELC: Should changes in concentration be printed? (1:yes, 0:no).

NPNCHV: Option to write velocity data on unit 7 (0, 1 or 2).

PINT: Length of pumping period in years.

TIMX: Time increment multiplier for transient flow problems.

TINIT: Size of initial time in seconds for transient flow problems.

10. Random-Walk Solute Transport Model

This program provides simulations of a large class of groundwater solute transport problem including the convection, dispersion, and chemical reactions. The solutions for groundwater flow include a finite-difference formulation. The solute transport portion of the code is based on a particle-in-a-cell technique for the convective mechanisms, and a random-walk technique for the dispersion effects.

The code can simulate one- or two-dimensional unsteady/steady flow problems in heterogeneous aquifers under water table and/or artesian or leaky artesian conditions. Furthermore this program covers time-varying pumpage or injection by wells, natural or artificial recharge, the flow relationships of water exchange between surface waters and the groundwater reservoir, the process of groundwater evapotranspiration, the mechanism of possible conversion of storage coefficients from artesian to water table conditions, and the flow from springs.

In addition, the program allows specification of chemical constituent concentrations of any segment of the model including, but not limited to, injection of contaminated water by wells, vertically averaged salt-water fronts, leachate from landfill, leakage from overlying source beds of differing quality than the aquifer, and surface water sources such as contaminated lakes and streams. The program documentation can be found in the following report: Prickett, T. A., T.G. Naymik, and C.G. Connquist, 1981, A "Random-Walk" solute transport model for selected groundwater quality evaluations, Bulletin 65, Illinois State Water Survey, Champaign, Illinois, 103 pages.

The **limitations** of RANDOM WALK are:

(1) As with MOC, concentrations greater than initial conditions are possible, especially when coarse discretizing is used.

(2) The method may take an unusually large number of particles to produce an acceptable solution for some problems (a maximum of 5,000 particles).

(3) Engineering judgment is an absolute requirement in arriving at an acceptable solution. This is because of the "lumpy" character of the output. Therefore, experience with this technique is needed before one can apply the code successfully to a field situation.

An window-driven preprocessor, PREWALK, is included with the program to facilitate user friendly data entry and editing.

11. MODFLOW groundwater flow model

MODFLOW is a three-dimensional finite-difference ground-water flow model. It has a modular structure that allows it to be easily modified. Many new capabilities have been added to the original model. This version includes all the major capabilities that were documented as of January, 1992.

In MODFLOW, groundwater flow within the aquifer is simulated using a block-centered finite-difference approach. Layers can be simulated as confined,

unconfined, or a combination of confined and unconfined. Flow from external stresses, such as flow to wells, areal recharge, evapotranspiration, flow to drains, and flow through riverbeds, can also be simulated. The finite-difference equations can be solved using either the Strongly Implicit Procedure or Slice-Successive Overrelaxation. The computer program is written in a modular form. It consists of a main program and a series of highly independent subroutines called "modules." The modules are grouped into "packages." Each package deals with a specific feature of the hydrologic system which is to be simulated. This version of MODFLOW includes the following packages:

- BAS1 -- Basic Package
- BCF2 -- Version 2 of Block-Centered Flow Package
- RIV1 -- River Package
- DRN1 -- Drain Package
- WEL1 -- Well Package
- GHB1 -- General Head Boundary Package
- RCH1 -- Recharge Package
- EVT1 -- Evapotranspiration Package
- SIP1 -- Strongly Implicit Procedure Package
- SOR1 -- Slice Successive Over-Relaxation Package
- UTL1 -- Utility Package
- PCG2 -- Version 2 of Preconditioned Conjugate Gradient Package
- STR1 -- Stream Package
- IBS1 -- Interbed Storage Package
- CHD1 -- Time-Variant Specified-Head Package
- GFD1 -- General Finite Difference Flow Package

The basic model is documented in: McDonald, M.G. and Harbaugh, A.W., 1988, A modular three-dimensional finite-difference ground-water flow model: U.S. Geological Survey Techniques of Water-Resources Investigations Book 6, Chapter A1, 586 pages. The PCG2 Package is documented in: Hill, M.C., 1990, Preconditioned conjugate-gradient 2 (PCG2), a computer program for solving ground-water flow equations: U.S. Geological Survey Water-Resources Investigations Report 90-4048, 43 pages. The STR1 Package is documented in: Prudic, D.E., 1989, Documentation of a computer program to simulate stream-aquifer relations using a modular, finite-difference, ground-water flow model: U.S. Geological Survey Open-File Report 88-729, 113 p. The IBS1 and CHD1 Packages are documented in: Leake, S.A. and Prudic, D.E., 1988, Documentation of a computer program to simulate aquifer system compaction using the modular finite-difference ground-water flow model: U.S. Geological Survey Open-File Report 88-482, 80 pages. The GFD1 Package is documented in: Harbaugh, A.W., 1992, A generalized finite-difference formulation for the U.S. Geological Survey modular three-dimensional finite-difference groundwater flow model: U.S. Geological Survey Open-File Report 91-494, 60 pages. The BCF2 Package is documented in: McDonald, M.G., Harbaugh, A.W., Orr, B.H., and Ackerman, D.J., 1992, A method of converting no-flow cells to variable-head cells for the U.S. Geological

Survey modular finite-difference ground-water flow model: U.S. Geological Survey Open-File Report 91-536, 99 pages.

The Main program has been modified to include all the packages. The IUNIT assignments for packages not in the original model are:

BCF -- IUNIT(1) -- same IUNIT as used for BCF1 because BCF2 replaces BCF1.
PCG2 -- IUNIT(13), GFD1 -- IUNIT(14), STR1 -- IUNIT(18), IBS1 -- IUNIT(19),
CHD1 -- IUNIT(20).

The input unit for the Basic package is unit 5, which is defined by the assignment of variable INBAS in the MAIN program.

The X array is dimensioned to 350,000. This is large enough for a model having approximately 20,000 cells.

The approximations applied to the flow equation to simulate the effects of a water table (water-table transmissivity calculation, vertical leakage correction, and confined/unconfined storage conversion) were developed using the conceptualization of a layered aquifer system in which each aquifer is simulated by one model layer and these aquifer layers are separated by distinct confining units. If one attempts to use the water-table transmissivity calculation in the situation where several model layers are simulating the same aquifer and the water table is expected to traverse more than one layer, problems with cells incorrectly converting to no flow may occur. Because the conversion to no flow is irreversible, only declines in the water table can be simulated. Vertical conductance is left constant until a cell converts to no flow, and then is set to zero. This assumes there is a confining layer, which dominates vertical flow, below the model water-table layer. In particular, the model program may have difficulty handling a multilayer simulation of a single aquifer in which a well causes drawdown below the top model layer. The solver may attempt to convert cells to no flow cells sooner than it should. This could cause the simulation to degenerate.

A shell program is provided for executing the program. The following files are for the example obtained from the original documentation:

twri.5	BAS1 Package input
twri.11	BCF2 Package input
twri.12	WEL1 package input
twri.13	DRN1 Package input
twri.18	RCH1 Package input
twri.19	SIP1 Package input

12. SUTRA

SUTRA (Saturated-Unsaturated Transport) is a computer program which simulates fluid movement and transport of either energy or dissolved substances in a subsurface environment. The model employs a two-dimensional hybrid finite-element and integrated-finite-difference method to approximate the governing equations that describe the two interdependent processes that are simulated:

- (1) fluid density-dependent saturated or unsaturated ground-water flow, and either
 - (2a) transport of a solute in the ground water, in which the solute may be subject to: equilibrium adsorption on the porous matrix, and both first-order and zero-order production or decay,
 - (2b) transport of thermal energy in the ground water and solid matrix of the aquifer.

SUTRA may be employed in one- or two-dimensional analyses. Flow and transport simulation may be either steady-state which requires only a single solution step, or transient which requires a series of time step in the numerical solution. Single-step steady-state solutions are usually not appropriate for non-linear problems with variable density, saturation, viscosity and non-linear sorption.

SUTRA flow simulation may be employed for areal and cross-sectional modeling of saturated groundwater flow systems, and unsaturated zone flow. Some aquifer tests may be analyzed with flow simulation. SUTRA solute transport simulation may be employed to model natural or man-induced chemical species transport including processes of solute sorption, production and decay. Such simulation may be used to analyze ground-water contaminant transport problems and aquifer restoration designs. SUTRA solute transport simulation may also be used for modeling of variable density leachate movement, and for cross-sectional modeling of salt-water intrusion in aquifers at both near-well or regional scales with either dispersed or relatively sharp transition zones between fresh and salt water. SUTRA energy transport simulation may be employed to model thermal regimes in aquifers, subsurface heat conduction, aquifer thermal energy storage system, geothermal reservoirs, thermal pollution of aquifers, and natural hydrogeologic convection system.

SUTRA will provide clear, accurate answers only to well posed, well-defined, and well-discretized simulation problems. In less-well-defined systems, SUTRA simulation can help visualize a conceptual model of the flow and transport regime, and can aid in deciding between various conceptual models. In such less-well-defined systems, simulation can help answer questions such as : Is the (inaccessible) aquifer boundary which is (probably) ten kilometers offshore either leaky or impermeable? How leaky? Does this boundary affect the primary analysis of onshore water supply?

SUTRA is not useful for making exact prediction of future responses of the typical hydrologic systems which are not well defined. Rather, SUTRA is useful for hypothesis testing and for helping to understand the physics of such a system. On the other hand, developing an understanding of a system based on simulation analysis can help make a set of worthwhile predictions which are predicated on uncertainty of both the physical model design and model parameter values. In particular, transport simulation which relies on large amounts of dispersion must be considered an uncertain basis for prediction, because of the highly idealized description inherent in the SUTRA dispersion process. A simulation-based prediction made with certainty is often inappropriate, and an "if-then" prediction is more realistic. In some cases, the available real data on a system may be so poor that a simulation using SUTRA is so ambiguously defined that no prediction at all can be made. In this instance, the simulation may be used to advantage in visualizing possible regimes of system behavior rather than to determine which is accurate.

In this UNIX version, a preprocessor for SUTRA has been developed. The preprocessor automatically generates input data files and a simulation units assignment file called SUTRA.FIL needed for running SUTRA. There are five set of files in this package:

- (1) preprocessor of SUTRA (presutra.f);
- (2) SUTRA main routines (main.f);
- (3) 24 SUTRA subroutines contained in three files: (a) USUBS.FOR, with two user-programmable routines, and (b) SUBS1.FOR and SUBS2.FOR with all the other subroutines;
- (4) two mesh data generation routines (mgenrec.f and mgenrad.f);
- (5) one routine for calculation of hydrostatic pressure dataset as specified pressure boundaries (pbcgen.f).

Reference materials for the original releases of these codes are:

Voss, Clifford I., 'A finite-element simulation model for saturated-unsaturated fluid-density-dependent groundwater flow with energy transport or chemically reactive single-species solute transport', U.S. Geological survey, Water-Resources investigations Report 84-4369, 1984.

13. Optim: Optimization of Remediation Design Program

This program provides an optimization design of pump-and-treat Remediation scheme, including the optimal well locations, pumping rates, and cost analysis. First of all, the main program extracts aquifer flow and contaminant characteristics from files created by running MOC for a present day model of the

groundwater contamination. The user is asked to enter the minimum acceptable contaminant concentration in order that a contaminant plume may be defined. In addition, the user enters the location of an observation well and a time frame for the Remediation effort. The observation well may be a domestic well or other point of contaminant level concern. The user may choose to locate the pumping well(s) manually or automatically. The user may choose any number of different remediation schemes to be considered and, if the manual location option is chosen, the number of wells in each scheme. If the user chooses to have the wells automatically located, a choice is made between an areal or a hydraulic barrier remediation approach. Following the location of the wells, the pumping rates are assigned, either manually or automatically, to each well. The cost of each remediation scheme is calculated. Finally, for each remediation scheme, the location of the wells, pumping rates, radii of influence, and cost are printed. Figure 56 shows an example contaminant plume and Figure 57 presents the areal control optimal pumping well locations calculated from Optim.

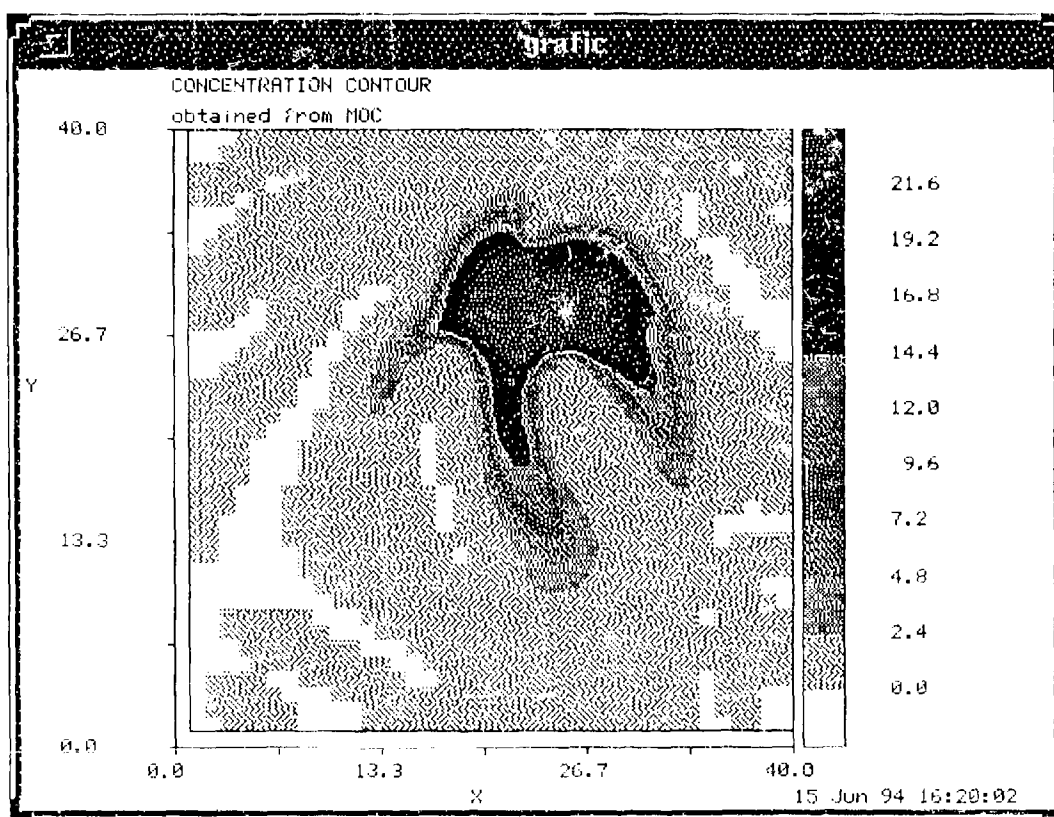


Figure 56. Contaminant contours simulated by MOC.

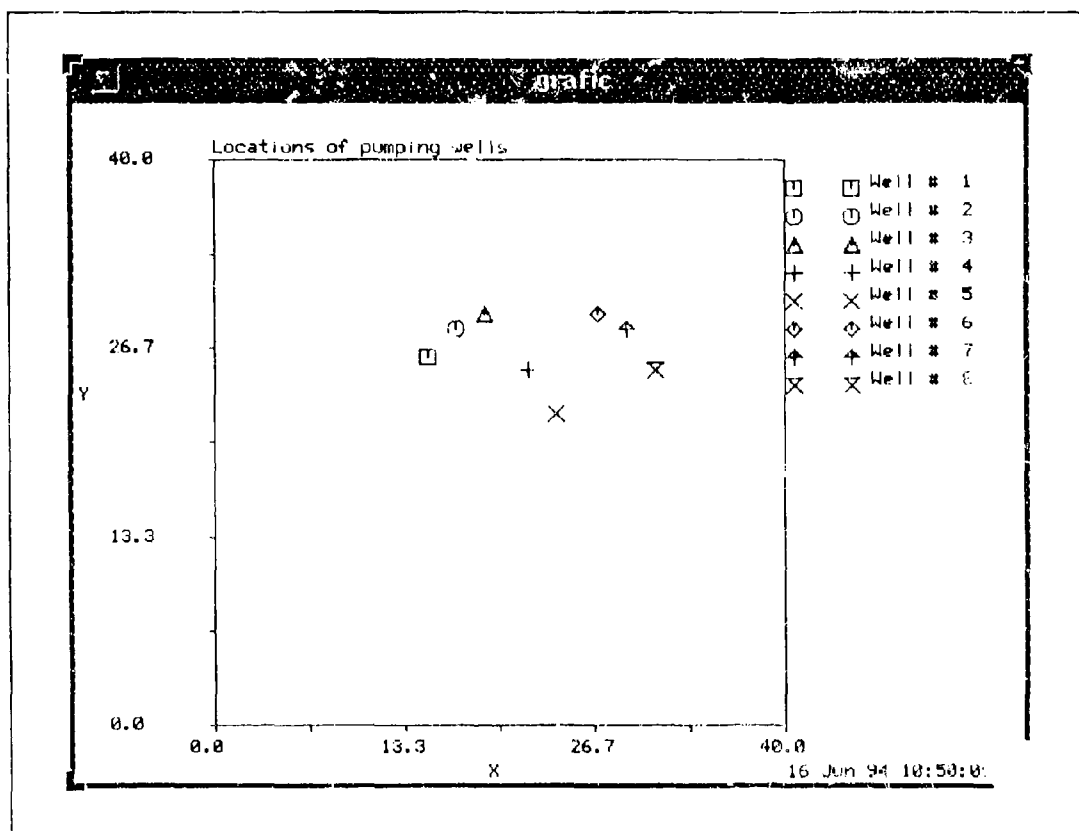


Figure 57. optimal pumping well locations calculated by optim.

This program gives the following information concerning remediation strategy:

a. Well locations

There are two options: an areal remediation scheme and a hydraulic barrier remediation scheme. If the areal remediation scheme is chosen, the X coordinates of the wells are assigned by the following equation:

$$X(j) = MinX + \frac{DimX}{2i} (2j - 1) \quad (25)$$

where X is the x coordinate of well j, i is the number of wells in the remediation scheme,

MinX is the minimum x coordinate of the contaminant plume, and DimX is the maximum dimension of the plume in the x direction. The above equation locates the wells equidistant over the length of the plume in the x direction. The Y coordinates of the wells are assigned by finding the dimension of the plume in the y direction at X(j). The well is then located in the center of the y plume dimension at the x coordinate of the well.

If the hydraulic barrier remediation scheme is chosen, the wells are located in a line such that they create a hydraulic wall toward which the contaminants flow. The wells extend perpendicular to the primary direction of flow between the contaminant plume minimum and maximum points in the direction parallel to flow. The equation for locating wells given flow in the +x direction is as follows:

$$X(j) = \text{MaxX} - \frac{\text{DimX}}{2j} \quad (26)$$

$$Y(j) = \text{MinY} + \frac{\text{DimY}}{2j} (2j - 1) \quad (27)$$

where MaxX is the maximum x coordinate of the contaminant plume and DimY is the maximum dimension of the plume in the y direction.

(2) Pumping rates

Pumping rates are chosen manually by the user or calculated automatically by the program for each well based on a radius of influence. For automatic calculation of pumping rates, the desired radius of influence was assumed to be one-half of the distance to the closest well. The MOC model makes the following assumption based on storage coefficient, S, about whether an aquifer is confined or unconfined (Konikow, 1978):

if $S < 0.005$ then assume $\partial b / \partial t = 0 \Rightarrow$ confined aquifer

if $S \geq 0.005$ then assume $\partial b / \partial t = \partial h / \partial t \Rightarrow$ unconfined aquifer

The following is the equilibrium pumping rate equation from a confined aquifer (DeMarsily, 1986):

$$Q = 2\pi T \frac{(H - h)}{\ln(R/r)} \quad (28)$$

where T is the transmissivity, H is the hydraulic head prior to pumping, h is the hydraulic head in the vicinity of the well borehole, R is the radius of influence of the well, and r is

the radius of the borehole. The equilibrium equation for an unconfined aquifer is calculated as:

$$Q = \pi K \frac{(H^2 - h^2)}{\ln(R/r)} \quad (29)$$

where K is the hydraulic conductivity ($T=Kb$). Sixty-seven percent drawdown is the maximum economical well operation since approximately 90 percent of a well's yield is achieved at 67 percent drawdown (Driscoll, 1986). However, the drawdown may vary with the radius of influence, an approximate way of calculating pumping rates without knowing the drawdown and influence radius is through the desired Darcy velocity along the boundary of influence radius:

$$Q = 2\pi Rbv \quad (30)$$

where R is the influence radius, b is the depth of aquifer, v is the flow velocity along the edge of the influence circle.

(3) Cost analysis

The cost of drilling is estimated to be 20 per vertical linear foot (Waier, 1992). The cost of pumps is related to the horsepower of the pump. For each well, the horsepower of the pump is calculated based on the total dynamic head, pump efficiency, and the pumping rate (Driscoll, 1986). The total dynamic head is assumed as the depth from the surface to the center of the saturated thickness of the aquifer. The pump efficiency is assumed to be 65 percent.

Since the program is based on the Thiem (equilibrium) equation, it cannot be applicable except within reasonable distances of a well. In another word, steady radial flow to a well is only achieved near the well where the hydraulic conductivities are homogeneous. Therefore, it is less accurate when applied to a case where large amount of contaminant exists and a very high pump rate is needed. Bear this in mind, the user should consider this program as a tool of visualizing the possible remediation schemes rather than obtaining some precise features of pump-and-treat system.

This model is designed as an interactive program, the user has to input the data for each prompt ask. First of all, this program needs the following data produced from running MOC:

var.dat, trans.dat, thck.dat, conc.dat

Besides that, the following data are needed:

1. The maximum concentration level of contaminant, MCL.
2. The desired location of observation well.
3. The remediation time frame (years).
4. The pumping well locations (if want to choose manually).
5. The number of remediation schemes.
6. Select areal remediation scheme or hydraulic barrier scheme.
7. The maximum pumping rate (gpm).
8. The diameter of pumping wells (inch).
9. The radii of influence or pumping rate (if want to choose manually).
10. The groundwater flow along the edge of the influence circle.
11. The depth to the aquifer.

14. Relib1d2

This program demonstrates the usefulness of the FOSM method for evaluating the reliability of specific groundwater contaminant remediation scenarios, a one-dimensional advection-diffusion example for nonreactive dissolved constituents in saturated, homogeneous, isotropic media under steady-state, uniform flow is presented. Mathematically, one-dimensional transient groundwater pollutant transport is defined as:

$$D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} \quad (31)$$

and subject to the boundary conditions :

$$\begin{aligned} C(x, 0) &= 0, \quad x \geq 0 \\ C(0, t) &= C_0, \quad t \geq 0 \\ C(\infty, t) &= 0, \quad t \geq 0 \end{aligned}$$

The analytical solution of Equation (31) can be obtained by using the Laplace transformation or other mathematical methods, it is in the form :

$$\frac{C}{C_0} = 0.5 \left\{ \operatorname{Erfc} \left(\frac{x - vt}{2\sqrt{Dt}} \right) + \exp \left(\frac{vx}{D} \right) \operatorname{Erfc} \left(\frac{x + vt}{2\sqrt{Dt}} \right) \right\} \quad (32)$$

where C_0 , C and x represent source concentration, the contaminant concentration at

time t and the distance downstream from the sources, respectively. The velocity, v of the groundwater is described using Darcy's formula ($v = k i$, where k represents hydraulic conductivity, and i the hydraulic gradient), D represents the longitudinal dispersion coefficient, as a function of the dispersivity within the groundwater media ($D = v a$, where " a " represents the dispersivity). The dispersivity is assumed to follow a normal distribution and the hydraulic conductivity follows a lognormal distribution. The Taylor expansion of the contaminant concentration, C , with respect to the mean of the dispersivity and the natural log of hydraulic conductivity is defined as:

$$C = C(\mu_a) + \frac{\partial C}{\partial a} (a - \mu_a) + \frac{\partial C}{\partial [\ln(k)]} (\ln(k) - \mu_{\ln(k)}) + \frac{\partial^2 C}{\partial a^2} \frac{(a - \mu_a)^2}{2} + \frac{\partial^2 C}{\partial [\ln(k)]^2} \frac{(\ln(k) - \mu_{\ln(k)})^2}{2} + O(\text{err}^3) \quad (33)$$

Ignoring the higher-order terms, the approximate mean and variance of the contaminant concentration, C , are defined with respect to the probabilistic model parameters..

In the case where both hydraulic conductivity and dispersivity are modeled as random variable, the mean and variance of the contaminant concentration is defined as:

$$\mu_C = C(\mu_a, \mu_{\ln(k)}) \quad (34)$$

and

$$\text{Var}(C) = \left(\frac{\partial C}{\partial a} \right)^2 \text{Var}(a) + \left(\frac{\partial C}{\partial [\ln(k)]} \right)^2 \text{Var}(\ln(k)) \quad (35)$$

For both cases, the partial derivatives $\partial C / \partial a$ and $\partial C / \partial [\ln(k)]$ are defined as:

$$\frac{\partial C}{\partial a} = \frac{C_0}{2} \left(\frac{ikt (ikt + x)}{2e^{\frac{x}{a} \frac{(ikt+x)^2}{4aikt}} \sqrt{\pi} (aikt)^{\frac{3}{2}}} - \frac{e^{\frac{x}{a} \frac{(ikt+x)^2}{4aikt}} \frac{ikt (ikt+x)}{2\sqrt{\pi} (aikt)^{\frac{3}{2}}} - \frac{e^{\frac{x}{a} \frac{(ikt+x)^2}{4aikt}} \operatorname{Erfc} \left(\frac{ikt+x}{2\sqrt{aikt}} \right)}{a^2} \right) \quad (36)$$

and

$$\frac{\partial C}{\partial [\ln(k)]} = \frac{C_0 k}{\sqrt{\pi}} \left(\frac{2 \left(\frac{ikt}{2\sqrt{aikt}} + \frac{ait (ikt+x)}{4(aikt)^{\frac{3}{2}}} \right)}{e^{\frac{x}{a} \frac{(ikt+x)^2}{4aikt}}} - \frac{e^{\frac{x}{a} \frac{(ikt+x)^2}{4aikt}} \left(\frac{ikt}{2\sqrt{aikt}} + \frac{ait (ikt+x)}{4(aikt)^{\frac{3}{2}}} \right)}{e^{\frac{x}{a} \frac{(ikt+x)^2}{4aikt}}} \right) \quad (37)$$

It is important to note that, both $\partial C / \partial [\ln(k)]$ and $\partial C / \partial a$ are evaluated at the mean values of a and $\ln(k)$.

The estimation of the mean and variance value of concentration using Monte Carlo simulation is also presented in the program to compare it with FOSM method. This program considers one-dimensional flow only. It evaluates the uncertainty of contaminant concentration under two major uncertain model parameters, hydraulic conductivity and dispersivity. However, it can be implemented into cases with more than two parameters using the same approach as presented above.

The information required by this program includes:

- (1) The value of initial concentration.
- (2) The magnitude of hydraulic gradient.
- (3) The contaminant release time (day).
- (4) The down-gradient of the source (m).
- (5) Number of Monte Carlo simulations.
- (6) Mean and standard deviation of conductivity (m / day)
- (7) Mean and standard deviation of dispersivity (m).

15. Relib1d

A reliability contour is constructed in this program using the same method mentioned in the previous section. There are three different reliability contours that can be obtained: time-distance related reliability contour, the distance-MCL (Maximum Concentration Level) related reliability contour, and the time-MCL related reliability contour. The user can choose either one of these three options.

The **limitations** of Relib1d are the same as in previous section.

The data needed for this program are:

- (1) The value of hydraulic gradient.
- (2) The value of initial concentration.
- (3) Type of reliability contour, there are three options:
 - a. Distance-Time contour with fixed MCL,
 - b. Distance-MCL contour with fixed Time,
 - c. Time-MCL contour with fixed Distance.

SECTION V

OPERATING SYSTEM CONSIDERATIONS

A. THE DOS ENVIRONMENT

Instructions related to the installation of both the DOS and UNIX versions of the software are presented in Section II, as well as a discussion of the basic features of the two operating systems as they relate to such installation. Other technical programming considerations are presented in this section.

1. DOS AND THE PERSONAL-COMPUTER ENVIRONMENT

This section provides technical notes relative to the method of programming. These notes are intended to be sufficiently detailed so that an experienced programmer would be able to readily extend, modify or adapt the system.

Recent advances in the power and affordability of the personal-computer (PC) have revolutionized the practice of pollutant transport modeling. Now, all but the most complex groundwater models can be run on personal computers and laptops (with expanded memory), freeing the user from reliance on mainframe computers. This increases the potential portability and availability of modeling systems, and the current system is designed with these goals in mind.

For maximum portability, the Advisory System is designed to run on personal computers that use the MS-DOS standard. DOS (Disk Operating System) is the command system which controls operations for the vast majority of these types of computers. The software has been tested up to MS-DOS Version 6.2 on IBM, Dell, Compaq and Toshiba computers with 386DX, 486DX, 486DX2 and Pentium chips, and up to 66 MHz clock speed. The system should be fully operational on any system that uses a DOS version 6.0 or higher with at least 4MB of RAM (although 8MB are recommended for the more complex stochastic simulations). The developers have endeavored to design the System, as far as possible, to run on any brand of personal computer that operates under DOS, given sufficient available memory and the presence of a fixed disk drive. As noted, a math co-processor is essential, as well as expanded memory.

A schematic of PC memory is presented in Figure 58. Conventional memory starts at 0K and normally ends at 640K (where most DOS programs run). In fact, most DOS programs until recently ran in *real mode*, with access only to the first megabyte (MB) of memory addresses (0-1024K). Upper memory starts at the end of conventional

memory and ends at 1024K. Upper memory is set aside for system ROM (Read-Only-Memory), video RAM (Random-Access-Memory), and BIOS (Basic Input Output System). Extended memory is the memory addressed above 1024K (used by programs operating in **protected** mode, such as Microsoft Windows). High memory area (HMA) is the first 64K of extended memory. With the newer DOS versions, part of the DOS operating system can be loaded in HMA. Expanded memory (EMS) is memory outside the first megabyte of PC memory that an expanded memory manager (e.g., EMM or QEMM) can cause to appear within the first MB in 16K units called **pages**.

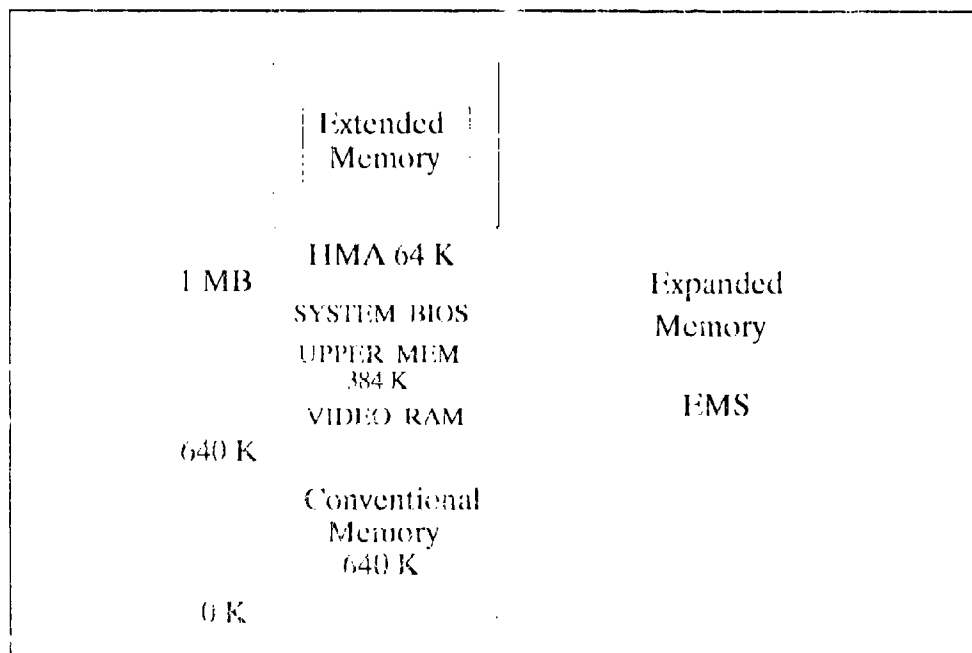


Figure 58. Basic PC Memory

Both DOS and availability of RAM memory limit the size of executable files to be used in the System. Because of this limitation, the System is designed in a modular fashion, and consists of many separate executable segments which are linked at the DOS command level through the use of batch files. The design of the Advisory System will be discussed in some detail in the following section.

2. MODULAR DESIGN OF THE ADVISORY SYSTEM

The computer-based workstation provides mathematical modeling capabilities to simulate flow and contaminant mass transport at a site. The system assists in the

selection of the most appropriate prediction model. It also performs risk assessment, accounting for natural and parameter uncertainty in the predictions, and selects an appropriate remediation method and remedial strategy.

The **file management** structure of the system was created to maintain good communication among the different modules. The main idea of the design is to preserve a single integrated package. The menu and utility programs link modular programs and data files. Through modular design, each transport model includes three main components: the preprocessor, the main code, and the postprocessor. The user can prepare the data set and run the transport model in the shell program. In a complete simulation, both input and output files are created and stored under separate subdirectories. These subdirectories are named as DAT and OUT.

For complicated groundwater models, for example, USGS MODFLOW and SUTRA, several input files may be necessary. Therefore, a subdirectory is created for each package to maintain integrity and flexibility. In the subdirectory, a shell program is used to control the model execution and store the data files.

User Interfaces are created as a bridge between the user and the contaminant transport models. These interfaces are easy to learn, flexible to use, and clear to manage. These interfaces can be roughly divided into two parts. One is the shell program, which is a menu-driven interface controlled with a mouse for making selections. The other is the model preprocessor which is flexible in the modification of input data. There are several functions included in the shell program: (1) to get help files for instruction; (2) to start the preprocessor program; (3) to run the main transport code; (3) to use graphics packages for model output, and (4) to manage the input and output files. The preprocessor program is designed as an efficient tool for preparation and modification of the model data. It is simple and requires less time to learn. The major objective of the preprocessor is to provide the user an easy-to-use modeling environment, and to assist the user in preparing the input data.

For visualization of model results, graphics packages were written specifically for the component models in the system. Modeling results, such as breakthrough curves and cumulative distribution curves of concentration, are plotted on the screen for interpretation, or printed directly to hardware devices. The advantages of graphical display are obvious.

The total size of the files required in the system is now approaching 12 million bytes. For the System to be operational in a personal-computer environment, only a portion of the system can be loaded into memory at any given time. The Advisory System has been designed to overcome this limitation, while still preserving the appearance and "flow" of a single, integrated package. This is done through modular design. Only one executable module of the system is loaded at any one time. The current module is linked to the whole system through DOS batch files, while a special

file structure is maintained for communication.

The individual executable files required in running the system are linked together at the DOS level through **batch** files. The linkage at this level requires maintenance of a special file system, which will be described below. Returning from any task through DOS while the system is running is basically invisible to the user. The user is presented with a menu of options, distinguished by letters or brief names. Selection of one of these options results in the execution of a batch file, which in turn will call the appropriate executable files in their proper sequence. In each of these procedures a file called MODEL.BAT is written by the procedure in accordance with the user's choices to execute the selected transport model.

As noted above, the system actually consists of a number of independent executable modules, linked at the DOS command level. To make these function as a whole, communication is required between the various constituent models. This is accomplished through maintenance of a special file structure. In the course of a run of the system (analyzing a single site), three files will be used: one specific to the run and two specific to the site. These are TEMP.DMP, {sitid}.DAT and {sitid}.OUT, where {sitid} is the code designation of the site. All three files will be created or located and updated upon entering the system, and must be present for the system to operate.

TEMP.DMP is a brief, direct access file (LRECL=80, FORM= 'FORMATTED') which keeps track of the current analysis, and informs the modules of the system of the site-specific names of the other two files. The {sitid}.DAT files primarily serve to preserve parameter values from each model run so that they can be reloaded for future applications on the same site. For some complex models, such as MODFLOW, the input files are stored in a separate subdirectory for convenience. The {sitid}.OUT files are ordinary, sequential access files which record the results of all analyses of a site.

3. File Linkage Guide

In order to avoid limits on size of the executable file, the system is composed of a large number of smaller executable files. These in turn may be composed of a number of object files, each representing a source file. Modifications to the existing parts of the system may thus require modification of these source files, which must then be recompiled and linked. These are written in several programming languages.

The bulk of the system is programmed in FORTRAN, using both real mode and protected mode (expanded memory) versions of the compilers, both 16-bit and 32-bit versions. Many of these FORTRAN codes are linked to C code for graphics purposes. Although individual modules may be re-compiled for execution with or without use of the math coprocessors, all executable files requiring extensive mathematical operations are presently compiled to take advantage of the increased speed of the math co-processors.

Several files are currently written in Turbo PASCAL, and must be compiled using the Turbo PASCAL compiler, configured as appropriate to the graphics hardware present. Compiling these files requires the presence of the Turbo PASCAL compiler. Make files and source files are listed below for component models. The PASCAL files and system utility files are listed in Tables 6 and 7.

Make files and source files

1. ODAST

ODAST.MAK = ODAST.FOR + CPU_TIME.FOR
ODASTP.EXE = ODASTP.FOR

2. TDAST

TDAST.MAK = TDAST.FOR + CPU_TIME.FOR

3. PLUM2D

PLUM2D.MAK = PLUM2D.FOR + PLUM2D2.FOR + RAN.FOR + ANSI.FOR
EXYPLT1.MAK = EXYPLT1.FOR + MASK2.FOR + PLOT.FOR

4. DUPVG

DUPVG.MAK = DUPVG.FOR + CPU_TIME.FOR

5. EPAGW

EPAGW.MAK = EPAGW1.FOR + EPAGW2.FOR + PARAM.FOR +
SCRNC.FOR + RAN.FOR + ATT.FOR
SFPLOT1.EXE = SFPLOT.FOR
CUMFQ1.EXE = CUMFQ1.FOR

6. EPASF

EPASF.MAK = EPASF1.FOR + EPASF2.FOR + EPASF3.FOR + EPASF4.FOR
+ SCRNC.FOR + RAN.FOR + ATT.FOR

7. LTIRD

LTIRD.EXE = LTIRD.FOR

8. RESSQ

RESSQ.EXE = RESSQ.FOR
FLWLIN.EXE = FLWLIN.FOR

9. USGS MOC

PREMOC.MAK = PREMOC.FOR + ANSI.FOR + IBMPCFIL.FOR
MOCAD1.EXE = MOCAD1.FOR + PARLOD.FOR + VELO.FOR + MOVE.FOR +
OUTP1.FOR

10. RANDOM WALK

PRNDWLK.MAK = PRWLKAS.FOR + WLKFLAS.FOR + TOOLS.FOR
 RNDWLK.MAK = RNDWLK.FOR + RWALK2.FOR

11. MODFLOW

PREMOD.EXE = PREMOD.FOR + PREMOD.INC
 MAIN1.EXE = MAIN1.FOR + BAS1.FOR + BCF2.FOR + CHD1.FOR +
 DRN1.FOR + EVT1.FOR + GFD1.FOR + GH1.FOR + IBS1.FOR +
 PCG2.FOR + RCH1.FOR + RIV1.FOR + STR1.FOR + SIP1.FOR +
 SOR1.FOR + UTL1.FOR + WEL1.FOR

12. SUTRA

SUTRA.EXE = MAIN.FOR + USUBS.FOR + SUBS1.FOR + SUBS2.FOR

13. BIOPLUME II

DRIVER.EXE = DRIVER.FOR + CLRSCR.FOR + BIOP.FOR + VELO.FOR +
 GENPT.FOR + MOVE.FOR + CNCON.FOR

14. ODAST in Monte Carlo Mode

ODASTMC.MAK = ODASTMC.FOR + CPU_TIME.FOR

15. TDAST in Monte Carlo Mode

TDASTMC.MAK = TDASTMC.FOR + CPU_TIME.FOR

16. MOC in Monte Carlo mode

PREMOC.MAK = PREMOC3.FOR + ANSI.FOR + IBMPCFIL.FOR
 MOCMC.EXE = MOCMC.FOR + TRNCOV1.FOR + CNCON3.FOR +
 MOVE3.FOR + PARLOD3.FOR + RANS.FOR + SOLUTE.FOR +
 VELO3.FOR

Table 6. PASCAL files for shell programs and preprocessors

VODAST.PAS	POTAST.PAS	VTDAST.PAS
PTDAST.PAS	MDUPVG.PAS	PDUPVG.PAS
MLTIRD.PAS	PLTIRD.PAS	VRESSQ.PAS
PRESSQ.PAS	VMOC.PAS	RANWLK.PAS
MODFLOW.PAS	FEM.PAS	BIOPLUM.PAS
VODASTMC.PAS	PODASTMC.PAS	VTDASTMC.PAS
PTDASTMC.PAS	VMOCMC.PAS	RUNHELP.PAS

Table 7. System utility files

BANNER.FOR	DIRMENU.FOR	GWEXP.FOR
GWGATE.FOR	LGRD.FOR	OPTIM.FOR
SCEN.FOR	SCRNC.FOR	LIST.PAS
LISTFL.PAS	SCROLL.PAS	

B. THE UNIX ENVIRONMENT

The main difference between the UNIX and DOS versions of the Advisory System is the operating system. The UNIX version of the system exploits the multi-user capabilities of the UNIX system. The UNIX version provides the user with access and operational capabilities that greatly exceed those available in most computers running under DOS. However, these expanded capabilities come with a cost. The UNIX version of the Advisory System has been written to run on a Sun Microsystems SPARC 2 or greater workstation. In addition, the Advisory System requires the use of Open Windows version 2.1.1 or greater. Typically, these type of workstations are greater in size and expense. For example, the DOS of the system can easily be installed on a laptop computer with sufficient memory and disk space. To date, no laptop computers available run the UNIX operating system.

The UNIX version is easily modified to run on alternative workstations running UNIX. Consult your systems site specialist for specific details on how to run the Advisory System on workstations other than the Sun Microsystems SPARC series.

The UNIX version of the Advisory System requires 29.7 MB of disk space, at least 4 MB of RAM and a 25 MHz clock. The performance and speed of the Advisory System can be greatly enhanced with increased memory and clock speed. For example, a Sun Microsystems SPARC 10 with 64 MB of RAM and a 33 MHz clock will be able to execute the groundwater models and graphics interfaces within the system much faster.

The UNIX system provides the user with the ability to run the Advisory System simultaneously with other UNIX software applications, access the system remotely and manipulate multiple input and output files. Due to the multiuser abilities of the UNIX operating system, the user is able to run the advisory system in conjunction with other software packages. For example, while running a time intensive model in the Advisory System, the user can easily initiate other processes such as the mail routine or one of the many editors residing on the workstation. These new processes do not have to be associated with the Advisory System. In addition, the Advisory System menu window can even be closed during long model runs to make more room on the screen for other activities. However, if the user quits the Advisory System menu window, the system will

terminate and any partially complete model runs will be lost. For additional information concerning the use of the UNIX system, the reader is referred to any available UNIX text or the workstation users manual.

The UNIX version also uses "makefiles" to create and link each of the source code files. Each of these "makefiles" shows how the subroutines are linked. To list these files use the command "more": refer to Table 1 in subsection II(B) for a complete listing of all the subroutines, makefiles and data files.

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APPENDIX A
TECHNICAL SUPPLEMENT

A. Model Development

To analyze groundwater contamination under conditions of uncertainty, Monte Carlo simulation is the most common and direct way. Often, the use of Monte Carlo simulation can be computationally cumbersome, especially when considering large-scale numerical models, such as MOC or SUTRA. To reduce the computational effort required to evaluate the probability of remediation failure, a first-order second-moment method (FOSM) can be used. This Appendix presents the theoretical development of the FOSM formulation used to determine the reliability of remediation strategies for some of the models in the Advisory System.

1. Groundwater flow and transport model

The governing equations of groundwater flow and contaminant transport in the saturated zone is expressed by :

$$S \frac{\partial h}{\partial t} = \nabla \cdot (T \cdot \nabla h) - q(x, y, t) \quad (\text{A-1})$$

$$v = \frac{T \cdot \nabla h}{nb} \quad (\text{A-2})$$

$$R \frac{\partial c}{\partial t} = \nabla \cdot (D \cdot \nabla c) - \nabla \cdot (vc) - \frac{\partial q}{\partial nb} + \lambda R(c - c^*) \quad (\text{A-3})$$

and subject to the following boundary conditions:

$$\begin{aligned} c &= c_0, \text{ at } t = t_0 && (\text{initial condition}) \\ \frac{dc}{dx} &= 0, \text{ at } x = x_1 && (\text{boundary condition 1}) \\ c_1 &= \text{MCL}, && (\text{boundary condition 2}) \\ \int q(x, y, t) dt &= Q_{\max}, && (\text{safety discharge}) \\ \int q(x, y, t) dt &= Q_{\min}, && (\text{allowable injection}) \\ h_1(q) &= h_1^*, && (\text{minimum water level}) \\ h_1(q) - h_2(q) &= h_{12}^*, && (\text{minimum gradient}) \\ L_1 + v_1(q) &= u_{12}, && (\text{allowable velocity}) \end{aligned}$$

Table A-1 defines each of the variables used in the flow and transport equations. In reality, model parameters such as hydraulic conductivity (K), the dispersion coefficient (D), Darcy velocity (v), the retardation factor (R), porosity (n) and the boundary conditions (Co, dh(x), 'dx) exhibit uncertainty due to difficulty in on-site measurement. To compensate for this variability, these parameters can be modeled as random variables with known spatial probability distributions.

Table A-1. Parameters in Groundwater Models

S	Storativity
T	Transmissivity = K b
K	Hydraulic Conductivity
R	Retardation Factor
D	Dispersion Tensor
v	Seepage Velocity Vector
c, c', c*	Pollutant Concentration
n	Porosity
b	Aquifer Thickness
h	Hydraulic Head
q	Extraction/Injection Rate
λ	Decaying Factor

2. Finding the distribution of state variables

Once the spatial distribution of the model parameters are established, the state variables (hydraulic head and contaminant concentration) are determined from the physical model using a Taylor series expansion. Mathematically, this approximation is defined as:

$$C(p) = C(\mu_p) + \sum_{i=1}^n \frac{\partial C}{\partial p_i} (p_i - \mu_{p_i}) +$$

$$0.5 \sum_{i=1}^n \sum_{j=1}^n \frac{\partial^2 C}{\partial p_i \partial p_j} (p_i - \mu_{p_i}) (p_j - \mu_{p_j}) + O\{(p_i - \mu_{p_i})^3\} \quad (\text{A-4})$$

where C represents the state variable for pollutant concentration, p, p_i , p_j define the groundwater model parameters in groundwater model, and μ_p is mean value of p.

Ignoring higher order terms, the mean and variance of the contaminant concentration, C, with respect to the physical parameters p are defined as:

$$\mu(C) = \int_{-\infty}^{\infty} C(p) f_x(p) dp = C(\mu_p) \quad (\text{A-5})$$

$$\text{Var}(C) = \int_{-\infty}^{\infty} (C(p) - \mu(C))^2 f_x(p) dp$$

$$= \sum_{i=1}^n \sum_{j=1}^n \frac{\partial C}{\partial p_i} \text{Cov}(p_i, p_j) \frac{\partial C}{\partial p_j} \quad (\text{A-6})$$

where $\partial C / \partial p$ is the sensitivity of contaminant concentration, C to the model parameter, p. The sensitivity is either calculated directly using an analytical solution of the governing equation or indirectly using a numerical model. For the case of analytical solution, the gradient of C with respect to p is easy to compute, since C is known explicitly. The difficulty arises when the analytical solution for the contaminant concentration, C is not available. The most efficient way is to calculate the sensitivity implicitly through using the model equations.

Let L represents the formulations of the governing equation for the groundwater and contaminant transport model. At fixed time and place, L is function of C and p, while C is dependent of p. Since L equals zero, the substantial (total) derivative of L with respect to variable p also equals zero.

$$\{L\} = \{L(C(p), p)\} = 0 \quad (\text{A-7})$$

$$\left\{ \frac{DL}{Dp} \right\} = \left\{ \frac{\partial L}{\partial C} \right\} \left\{ \frac{\partial C}{\partial p} \right\} + \left\{ \frac{\partial L}{\partial p} \right\} = 0 \quad (\text{A-8})$$

Therefore, the sensitivity is determined by multiplying the inverse gradient matrix of L with respect to C and the gradient matrix of L with respect to p.

$$\left\{ \frac{\partial C}{\partial p} \right\} = - \left\{ \frac{\partial L}{\partial C} \right\}^{-1} \left\{ \frac{\partial L}{\partial p} \right\} \quad (\text{A-9})$$

Since the model's governing equations are second-order partial differential equations, it is not easy to differentiate the original differential equations with respect to the parameters of interest. Therefore, the numerical solving scheme (such as finite elements) is preferred in solving such stochastic groundwater contaminant transport problem. In a finite element algorithm, the numerical approximations of these essential governing equations are derived to form a set of discretized linear algebraic equations. Hence, the differentiation of these linear equations with respect to both the contaminant concentration C and the model parameter p is easily calculated. More details on this methodology are described in the numerical examples presented later in this Appendix.

Defining the mean and variance of the state (dependent) variables, the model variability is quantified using the coefficient of variation (COV),

$$\text{COV} = \left(\frac{\text{Var}(C)}{\mu(C)^2} \right)^{0.5} \quad (\text{A-10})$$

3. Probability of Remediation Strategy Failure

The probability of remediation failure is defined as the probability that the contaminant concentration exceeds the maximum allowable concentration level (MCL). Mathematically, the probability of failure is expressed as :

$$P_f = P(C > \text{MCL}) \quad (\text{A-11})$$

and reflects the probability that groundwater quality will not be maintained. For a specific remediation strategy, M is defined as the safety margin of groundwater quality :

$$M = MCL - C$$

(A-12)

Defining C as a random variable, M is also a random variable with a mean of $\mu_M = MCL - \mu_C$ and standard deviation $\sigma_M = \sigma_C = \sqrt{\text{Var}(C)}$. Since there is only one random variable in the performance function. The mean and variance of the Safety Margin are defined using a Taylor expansion. Noting that the performance function, equation (A-12) is invariant, the limit-surface addressed by Sitar (1987) does not need to be considered.

Failure occurs when the estimated contaminant concentration is greater than MCL :

$$M < 0$$

(A-13)

If the distribution of the contaminant concentration is assumed to follow a normal distribution, M can be scaled to have a mean of 0 and a standard deviation of 1. The reduced variate, M' , also follows a normal probability distribution and is defined as:

$$M' = \frac{M - \mu(M)}{\sigma(M)} = -\frac{C - \mu(C)}{\sigma(C)} \quad (\text{A-14})$$

Using the reduced variate, the probability of failure is evaluated in terms of the cumulative distribution. Mathematically, this is expressed as :

$$p_f = F_M(0) = \Phi\left(\frac{\mu(M)}{\sigma(M)}\right) = \Phi\left(-\frac{MCL - \mu(C)}{\sigma(C)}\right) \quad (\text{A-15})$$

where $F(\bullet)$ represents the cumulative distribution function, and $\Phi(\bullet)$ defines the standard probability density function. Equation (A-16) illustrates that the probability of failure is a function of the ratio:

$$\beta = \frac{\mu(M)}{\sigma(M)} = \frac{MCL - \mu(C)}{\sigma(C)} \quad (\text{A-16})$$

where β is often referred to as the *safety index*. Two important issues are worth mentioning here. First, the performance function, equation (A-12), has only one random variable; therefore,

the value of β is invariant. Secondly, with only second-moment information, the probability of failure cannot be estimated by either the Monte Carlo method or the FOSM method (at best, rather wide bounds can be estimated). The underlying assumption of this methodology is that the distribution of the contaminant concentration follows a normal distribution. Often, the probability distribution of the contaminant concentration and the resulting margin of safety do not follow a normal distribution. In such cases, the distribution of the concentration can be transformed into an equivalent normal distribution function using the Rosenblatt transformation (Ang and Tang [1984]). Using a Taylor series to approximate the mean and standard deviation of the contaminant concentration results in an approximation of the safety index, β . As a result, the corresponding probability of failure is also an approximation:

$$p_f = \Phi(-\beta) = 1 - \Phi(\beta) \quad (\text{A-17})$$

where $\Phi(i)$ is the standard normal cumulative probability evaluated at i .

4. Determining the Point Reliability

The reliability of not exceeding the MCL at any point on the contaminant site can be calculated as:

$$R_{ij} = 1 - p_f = p\{c_{ij} < MCL_i\} \quad (\text{A-18})$$

where i represents the location of a pumping well, and j represents the position of a monitoring well. Expressing the random variable in reduced variate form yields:

$$z = \frac{c_{ij} - \mu(c_{ij})}{\sigma(c_{ij})} \quad (\text{A-19})$$

Using the reduced variate form, the probability that the contaminant concentration will not exceed the MCL is defined as:

$$R_{ij} = p\left\{z \leq \frac{MCL_i - \mu(c_{ij})}{\sigma(c_{ij})}\right\} \quad (\text{A-20})$$

As a function of the cumulative probability function, $\Phi(\cdot)$, the probability of not exceeding the MCL is expressed as:

$$R_{ij} = \Phi \left\{ \frac{MCL_i - \mu(C_{ij})}{\sigma(C_{ij})} \right\} = \Phi(\beta_{ij}) \quad (A-21)$$

Consequently, the reliability of a pump-and-treat remediation strategy is directly related to the safety index, β . By assuming the resulting distribution of the contaminant concentration follows a normal distribution, the reliability of a specific remediation strategy can be estimated using only the mean and standard deviations of the contaminant concentration. As a result, using the FOSM method in estimating the reliability of the remediation strategy is much more efficient than using typical Monte Carlo simulations.

B. Numerical illustrations

In order to demonstrate the implementation of the methodology discussed here, three examples are presented. In the first example, a one-dimensional analytical groundwater model with one and two probabilistic parameters is studied and discussed. The second example is a two dimensional groundwater transport finite element numerical model with one and two model parameters as random variables. The third example is an extension of the second example with a heterogeneous random field.

1. Example one

To demonstrate the usefulness of the FOSM method for evaluating the reliability of specific groundwater contaminant remediation scenarios, a one-dimensional advection-diffusion example for nonreactive dissolved constituents in saturated, homogeneous, isotropic media under steady-state, uniform flow is presented. Mathematically, one-dimensional transient groundwater pollutant transport is defined by:

$$D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} \quad (A-22)$$

and subject to the boundary conditions :

$$C(x, 0) = 0, \quad x \geq 0$$

$$\begin{aligned} C(0, t) &= C_0, & t > 0 \\ C(\infty, t) &= 0, & t \geq 0 \end{aligned}$$

The analytical solution of equation (A-22) is obtained by using the Laplace transformation or other mathematical methods, and yields :

$$\frac{C}{C_0} = 0.5 \left\{ \operatorname{Erfc} \left(\frac{x - vt}{2\sqrt{Dt}} \right) + \operatorname{Exp} \left(\frac{vx}{D} \right) \operatorname{Erfc} \left(\frac{x + vt}{2\sqrt{Dt}} \right) \right\} \quad (\text{A-23})$$

where C_0 , C and x represent source concentration, the contaminant concentration at time t and the distance downstream from the sources, respectively. The velocity v of the groundwater is described using Darcy's formula ($v = k I$, where k represents hydraulic conductivity, and I the hydraulic gradient), D represents the longitudinal dispersion coefficient as a function of the dispersivity within the groundwater media ($D = v a$, where " a " represents the dispersivity).

For this illustrative example, only the dispersivity and hydraulic conductivity are modeled as random variables with known probability distributions. The dispersivity is assumed to follow a normal distribution and the hydraulic conductivity follows a lognormal distribution. The Taylor expansion of the contaminant concentration, C , with respect to the mean of the dispersivity and the natural log of hydraulic conductivity is defined as:

$$C = C(\mu_a) + \frac{\partial C}{\partial a} (a - \mu_a) + \frac{\partial C}{\partial [\ln(k)]} (\ln(k) - \mu_{\ln(k)}) +$$

$$\frac{\partial^2 C}{\partial a^2} \frac{(a - \mu_a)^2}{2} + \frac{\partial^2 C}{\partial [\ln(k)]^2} \frac{(\ln(k) - \mu_{\ln(k)})^2}{2} + O(\text{err}^3) \quad (\text{A-24})$$

Ignoring the higher order terms, the approximate mean and variance of the contaminant concentration, C , are defined with respect to the probabilistic model parameters.

In the case where only the hydraulic conductivity is modeled as a random variable, the mean and variance of the contaminant concentration is approximated as:

$$\mu_c = C(\mu_{\ln(k)}) \quad (A-25)$$

and

$$\text{Var}(C) = \left(\frac{\partial C}{\partial [\ln(k)]} \right)^2 \text{Var}(\ln(k)) \quad (A-26)$$

In the case where both hydraulic conductivity and dispersivity are modeled as random variable, the mean and variance of the contaminant concentration is defined as:

$$\mu_c = C(\mu_a, \mu_{\ln(k)}) \quad (A-27)$$

and

$$\text{Var}(C) = \left(\frac{\partial C}{\partial a} \right)^2 \text{Var}(a) + \left(\frac{\partial C}{\partial [\ln(k)]} \right)^2 \text{Var}(\ln(k)) \quad (A-28)$$

For both cases, the partial derivatives $\partial C / \partial a$ and $\partial C / \partial k$ are defined as:

$$\begin{aligned} \frac{\partial C}{\partial a} = & \frac{C_0}{2} \left(- \frac{ikt(-(ikt)+x)}{2e^{\frac{x}{a} \frac{-(ikt+x)^2}{4aikt}} \sqrt{\pi}(aikt)^{\frac{3}{2}}} + \right. \\ & \left. \frac{e^{\frac{x}{a} \frac{-(ikt+x)^2}{4aikt}}}{2\sqrt{\pi}(aikt)^{\frac{3}{2}}} \frac{ikt(ikt+x)}{a^2} \right) \quad (A-29) \\ & e^{\frac{x}{a} \frac{-(ikt+x)^2}{4aikt}} \text{Erfc} \left(\frac{ikt+x}{2\sqrt{aikt}} \right) \end{aligned}$$

and

$$\frac{\partial C}{\partial [\ln(k)]} = \frac{C_0 k}{\sqrt{n}} \left\{ \frac{2 \left(\frac{(it)}{2\sqrt{aikt}} + \frac{ait(-ikt)+x}{4(aikt)^{\frac{3}{2}}} \right)}{e^{\frac{(ikt+x)^2}{4aikt}}} - \frac{e^{\frac{x}{a} - \frac{(ikt+x)^2}{4aikt}} \left(\frac{it}{2\sqrt{aikt}} - \frac{ait(ikt+x)}{4(aikt)^{\frac{3}{2}}} \right)}{e^{\frac{(ikt+x)^2}{4aikt}}} \right\} \quad (A-30)$$

It is important to note that, both $\partial C/\partial a$ and $\partial C/\partial k$ are evaluated at the mean values of a and $\ln(k)$.

For this illustrative example, two simulation scenarios are considered. The first case consider only one random variable to illustrate the accuracy of the FOSM method. The second case is more complicated and involves two random variables. The second case presents a more realistic representation of the proposed method. Table A-2 presents the data for each scenario considered:

Table A-2. Parameters values used in the two case designs.

Parameter	Case 1			Case 2		
	set 1	set 2	set 3	set 1	set 2	set 3
$\mu_{\ln(k)}$	-3	-4	-5	-3	-4	-5
$\sigma_{\ln(k)}$	0.5	0.7	0.9	0.5	0.6	0.7
μ_a				40	60	30
σ_a				10	10	7

The first case assumes hydraulic conductivity k to be the only random variable following a lognormal distribution with mean $\mu_{\ln(k)}$ and standard deviation $\sigma_{\ln(k)}$. As shown in Table A-2, three different mean and variance values for k are examined and compared using the FOSM method and Monte Carlo simulation. The reliability-maximum concentration level (MCL) relationship resulting from the two methods illustrates a high degree of agreement (see Figures A-1, A-2 and A-3).

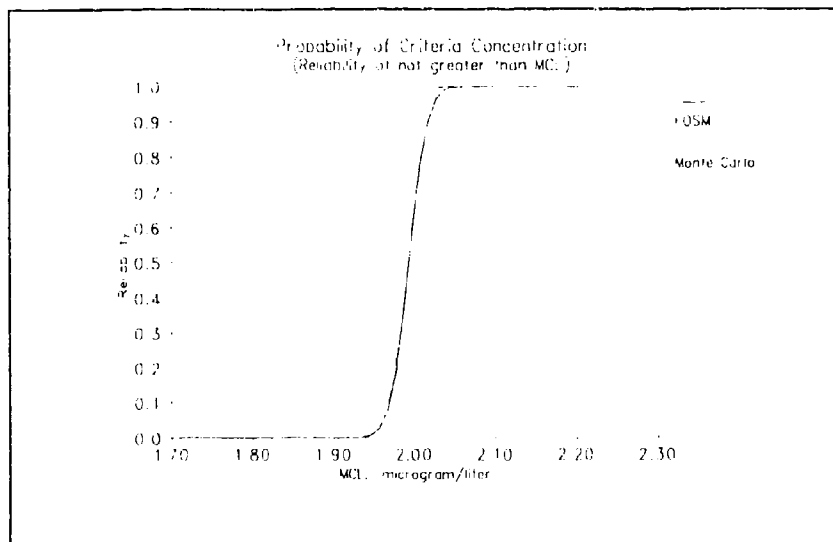


Figure A-1. Comparison of FOSM and Monte Carlo method, $\mu_{\ln(k)} = -3$, $\sigma_{\ln(k)} = 0.5$.

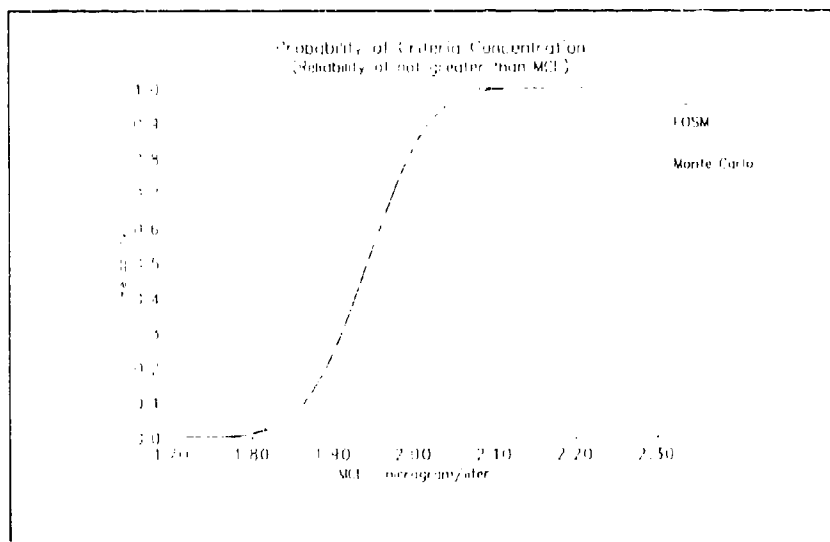


Figure A-2. Comparison of FOSM and Monte Carlo method, $\mu_{\ln(k)} = 4$, $\sigma_{\ln(k)} = 0.7$.

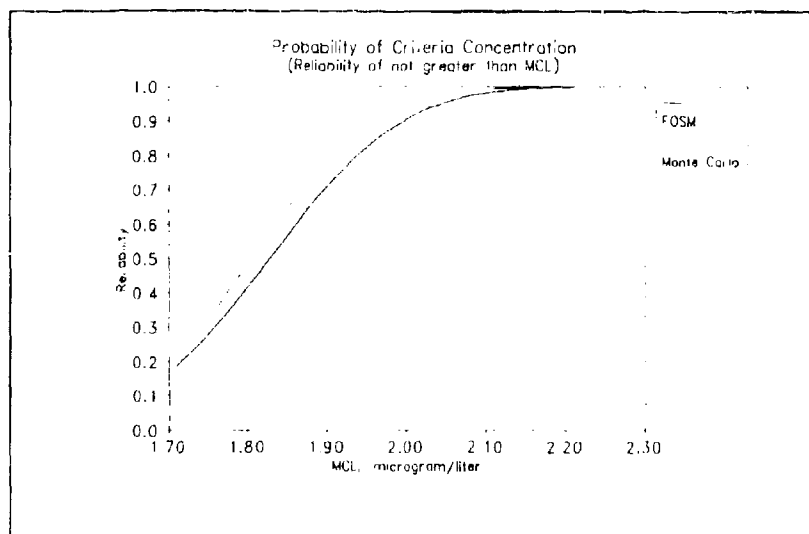


Figure A-3. Comparison of FOSM and Monte Carlo method, $\mu_{\ln(k)} = -5$, $\sigma_{\ln(k)} = 0.9$.

In the second case, both hydraulic conductivity, k , and dispersivity, a , are modeled as random variables. Three different sets of parameters are used in this case as presented in Table A-2. Again, the results presented in Figures A-4, A-5 and A-6 illustrate that the reliability-MCL relationship resulting from using the FOSM method closely resembles the results using Monte Carlo simulation. However, the results using the FOSM method with higher standard deviations for the random variables yield an increase in the skewness of the resulting cumulative distribution function (CDF).

Since the FOSM method can estimate the uncertainty of state variable appropriately with much less computational effort than the Monte Carlo simulations, this advantage can be exploited in constructing the reliability curves or contour associated with multiple decision factors (such as pollutants release time, monitoring well position, and MCL). Figures A-7, A-8 and A-9 illustrate the reliability contours constructed for multiple decision factors: pollutant release time, monitoring well position and MCL.

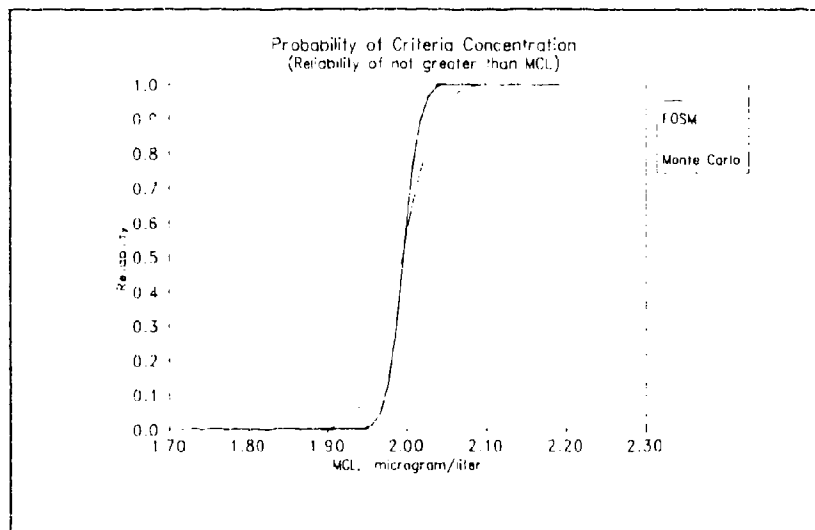


Figure A-4. Comparison of FOSM and Monte Carlo method, $\mu_{\ln(k)} = -3$, $\sigma_{\ln(k)} = 0.5$, $\mu_a = 40$, $\sigma_a = 10$.

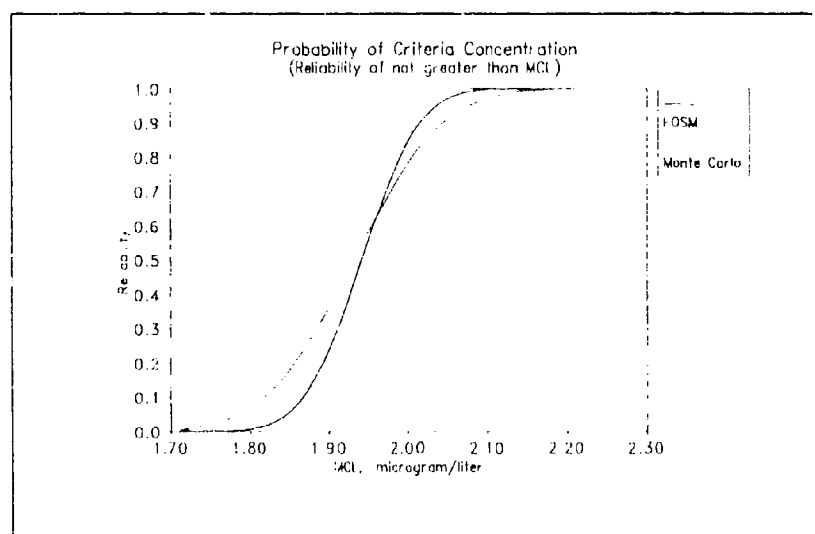


Figure A-5. Comparison of FOSM and Monte Carlo method, $\mu_{\ln(k)} = -4$, $\sigma_{\ln(k)} = 0.6$, $\mu_a = 60$, $\sigma_a = 10$.

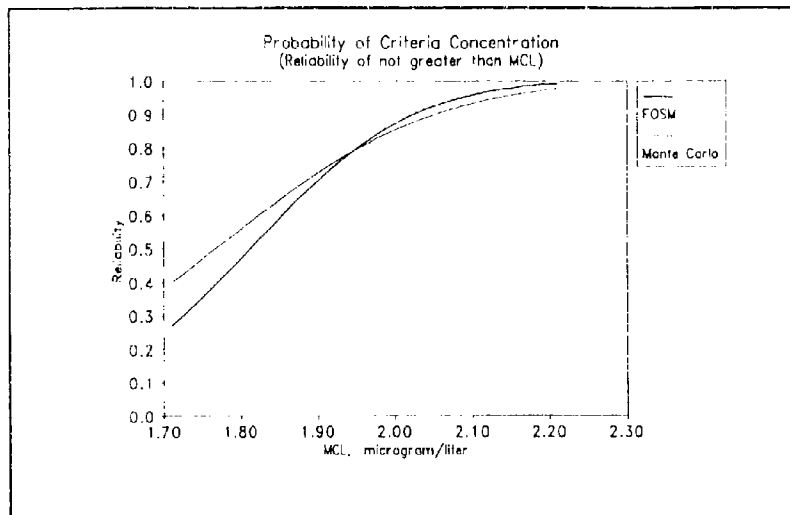


Figure A-6. Comparison of FOSM and Monte Carlo method, $\mu_{\ln(k)} = -5$, $\sigma_{\ln(k)} = 0.7$, $\mu_a = 30$, $\sigma_a = 7$.

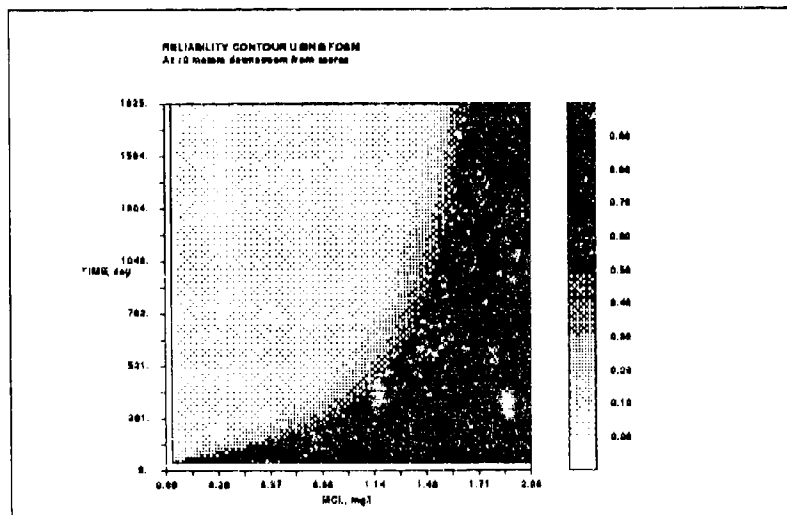


Figure A-7. Reliability contour under $\mu_{\ln(k)} = -5$, $\sigma_{\ln(k)} = 0.9$, $\mu_a = 30$, $\sigma_a = 7$.

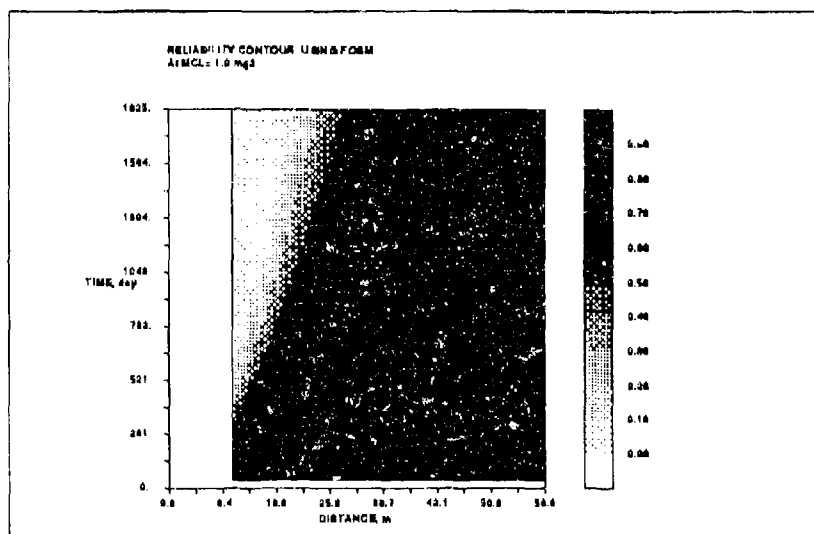


Figure A-8. Reliability contour under $\mu_{\ln(k)} = -5$, $\sigma_{\ln(k)} = 0.9$, $\mu_a = 30$, $\sigma_a = 7$.

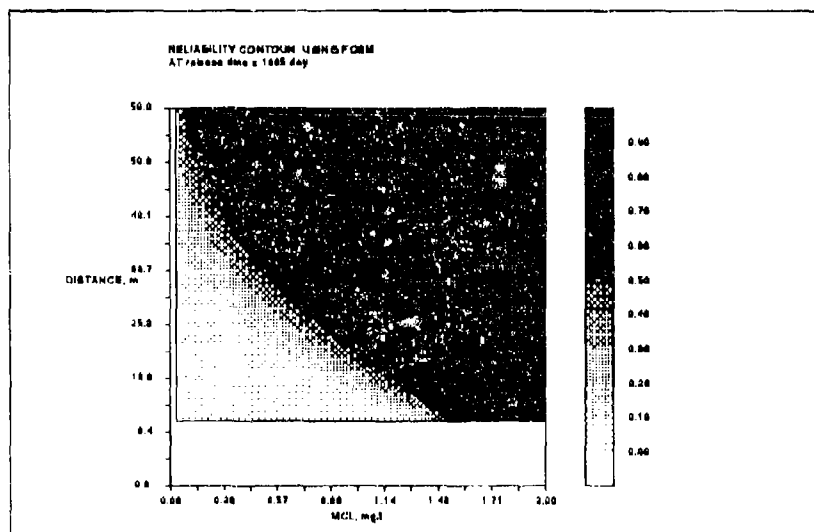


Figure A-9. Reliability contour under $\mu_{\ln(k)} = -5$, $\sigma_{\ln(k)} = 0.9$, $\mu_a = 30$, $\sigma_a = 7$.

In this illustration, the FOSM method is shown to be an efficient method for approximating the mean and standard deviation of contaminant concentration, and the reliability contour in a one-dimensional, transient state groundwater transport model, when one or more than one physical parameters is unknown.

2. Example two

The previous example shows the application of the FOSM method to the simple pollutant transport model using an analytical solution. In general, a real site is much more complicated and inappropriate for an analytical solution. Rather, a numerical solution is preferred. In this example, the FOSM method is applied to a more sophisticated problem using numerical solution. A two-dimensional advection-dispersion transport problem for a homogeneous medium in a uniform flow field with Dirichlet boundary condition is studied. The governing equation for this example is defined:

$$D_1 \frac{\partial^2 C}{\partial x^2} + D_t \frac{\partial^2 C}{\partial y^2} - v_x \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} \quad (\text{A-31})$$

where the groundwater flow follows Darcy's law (i.e. $v_x = k l$), and dispersion coefficients are assumed linear with v_x (i.e. $D_1 = a_1 v_x$, $D_t = a_t v_x$). As in example one, this example considers hydraulic conductivity, k , and the dispersion coefficients, a_1 , a_t , as random variables with log-normal and normal distributions, respectively.

Using a Galerkin approach, the integration over the problem domain becomes:

$$\begin{aligned} 0 = \int_{\Gamma} N_B D_{ij} \sum_A \left(\frac{\partial N_A}{\partial x_i} C_A \right) n_i d\Gamma - \int_{\Omega} \frac{\partial N_B}{\partial x_i} D_{ij} \sum_A \left(\frac{\partial N_A}{\partial x_j} C_A \right) d\Omega \\ + \int_{\Omega} N_B \left\{ -u_i \sum_A \left(\frac{\partial N_A}{\partial x_i} C_A \right) - \frac{\partial}{\partial t} \left(\sum_A N_A C_A \right) \right\} d\Omega \end{aligned} \quad (\text{A-32})$$

In matrix notation, the above system of equation is defined by:

$$\mathbf{G}\{\mathbf{C}\} + \mathbf{U}\{\mathbf{C}\} + \mathbf{P}\left\{\frac{\partial \mathbf{C}}{\partial t}\right\} = \{\mathbf{f}\} \quad (\text{A-33})$$

where \mathbf{C} is the column matrix of nodal concentrations, \mathbf{f} is the column matrix of the boundary integral and $\partial \mathbf{C} / \partial t$ is the column matrix of the time derivative of the nodal concentrations. The square coefficient matrices, \mathbf{G} , \mathbf{U} and \mathbf{P} correspond to the dispersion terms, advection terms and mass terms of the system, respectively. The element matrix entries for these coefficient matrices are defined as:

$$G_i^e = \int \int (D_i \frac{\partial N_i^e}{\partial x} \frac{\partial N_i^e}{\partial x} + D_i \frac{\partial N_i^e}{\partial y} \frac{\partial N_i^e}{\partial y}) dx dy \quad (A-34)$$

$$U_{1i}^e = v_x \int \int \frac{\partial N_i^e}{\partial x} N_i^e dx dy \quad (A-35)$$

$$P_{1i}^e = \int \int N_i^e N_i^e dx dy \quad (A-36)$$

The assembly of the global matrices is preformed by summing each element matrix within the system. Equation (A-33) is solved with respect to time using a finite difference approximation for $\partial C / \partial t$:

$$(\mathbf{G} + \mathbf{U} + \frac{\mathbf{P}}{\Delta t}) \{C\}^{t+\Delta t} = \frac{\mathbf{P}}{\Delta t} \{C\}^t + \{f\} \quad (A-37)$$

Letting L_i represents the i^{th} row of the matrix, equation (A-37), yields

$$L_i = (G_{1i} + U_{1i} + \frac{P_{1i}}{\Delta t}) C_i^{t+\Delta t} - \frac{P_{1i}}{\Delta t} C_i^t - f_i = 0 \quad (A-38)$$

For a fixed position and time, L_i is considered a function of C_i^t , $C_i^{t+\Delta t}$, v_x , and a , where C_i^t and $C_i^{t+\Delta t}$ are also function of v_x , and a . By definition, the substantial derivative of L_i equals zero. Applying the chain rule yields:

$$\frac{DL_i}{Dv_x} = \frac{\partial L_i}{\partial C_i^{t+\Delta t}} \frac{\partial C_i^{t+\Delta t}}{\partial v_x} + \frac{\partial L_i}{\partial C_i^t} \frac{\partial C_i^t}{\partial v_x} + \frac{\partial L_i}{\partial v_x} = 0 \quad (A-39)$$

$$\frac{DL_i}{Da} = \frac{\partial L_i}{\partial C_i^{t+\Delta t}} \frac{\partial C_i^{t+\Delta t}}{\partial a} + \frac{\partial L_i}{\partial C_i^t} \frac{\partial C_i^t}{\partial a} + \frac{\partial L_i}{\partial a} = 0 \quad (A-40)$$

Therefore, the column matrices of first partial derivatives of C with respect to v_x and a at time $t+\Delta t$ are defined as :

$$\left\{ \frac{\partial C_i^{t+\Delta t}}{\partial v_x} \right\} = - \left\{ \frac{\partial L_I}{\partial C_i^{t+\Delta t}} \right\}^{-1} \left\{ \frac{\partial L_I}{\partial v_x} + \frac{\partial L_I}{\partial C_i^t} \frac{\partial C_i^t}{\partial v_x} \right\} \quad (A-41)$$

and

$$\left\{ \frac{\partial C_i^{t+\Delta t}}{\partial a} \right\} = - \left\{ \frac{\partial L_I}{\partial C_i^{t+\Delta t}} \right\}^{-1} \left\{ \frac{\partial L_I}{\partial a} + \frac{\partial L_I}{\partial C_i^t} \frac{\partial C_i^t}{\partial a} \right\} \quad (A-42)$$

where

$$\frac{\partial L_I}{\partial C_i^{t+\Delta t}} = G_{Ii} + U_{Ii} + \frac{P_{Ii}}{\Delta t} \quad (A-43)$$

$$\frac{\partial L_I}{\partial v_x} + \frac{\partial L_I}{\partial C_i^t} \frac{\partial C_i^t}{\partial v_x} = - \frac{\partial (G_{Ii} + U_{Ii})}{\partial v_x} C_i^{t+\Delta t} + \frac{P_{Ij}}{\Delta t} \frac{\partial C_j^t}{\partial v_x} \quad (A-44)$$

and

$$\frac{\partial L_I}{\partial a} + \frac{\partial L_I}{\partial C_i^t} \frac{\partial C_i^t}{\partial a} = - \frac{\partial G_{Ii}}{\partial a} C_i^{t+\Delta t} + \frac{P_{Ij}}{\Delta t} \frac{\partial C_j^t}{\partial a} \quad (A-45)$$

For each element, $\partial (G_{Ii} + U_{Ii}) / \partial v_x$ and $\partial G_{Ii} / \partial a$ are defined as :

$$\begin{aligned} \frac{\partial (G_{Ii}^e + U_{Ii}^e)}{\partial v_x} &= \int \int (a_1 \frac{\partial N_i^e}{\partial x} \frac{\partial N_i^e}{\partial x} + a_t \frac{\partial N_i^e}{\partial y} \frac{\partial N_i^e}{\partial y}) dx dy \\ &+ \int \int \frac{\partial N_i^e}{\partial x} N_i^e dx dy \end{aligned} \quad (A-46)$$

$$\frac{\partial G_i^o}{\partial a_i} = \iint v_x \frac{\partial N_i^o}{\partial x} \frac{\partial N_i^o}{\partial x} dx dy \quad (A-47)$$

$$\frac{\partial G_{1i}^o}{\partial a_t} = \iint v_x \frac{\partial N_i^o}{\partial y} \frac{\partial N_i^o}{\partial y} dx dy \quad (A-48)$$

The assembly of the above terms into a global matrix is similar to the assembly of the matrices **G**, **U** and **P**. Finally, the mean and variance of $C_i^{t+\Delta t}$ are found to be :

$$\mu (C_i^{t+\Delta t}) = C_i^{t+\Delta t} (\mu (\ln(k)), \mu(a_1), \mu(a_t)) \quad (A-49)$$

$$\begin{aligned} \text{Var}(C_i^{t+\Delta t}) = & \left(\frac{\partial C_i^{t+\Delta t}}{\partial a_1} \right)^2 \text{Var}(a_1) + \left(\frac{\partial C_i^{t+\Delta t}}{\partial a_t} \right)^2 \text{Var}(a_t) \\ & + \left(\frac{\partial C_i^{t+\Delta t}}{\partial (\ln(k))} \right)^2 \text{Var}(\ln(k)) + \left(\frac{\partial C_i^{t+\Delta t}}{\partial a_1} \right)^2 \text{Var}(a_1) \\ & + \left(\frac{\partial C_i^{t+\Delta t}}{\partial a_t} \right)^2 \text{Var}(a_t) + \left(v_x \frac{\partial C_i^{t+\Delta t}}{\partial v_x} \right)^2 \text{Var}(\ln(k)) \end{aligned} \quad (A-50)$$

The solution algorithm of the mean and variance of contaminant concentration is broken into four steps:

- [1] Initialize $\partial C_i^0 / \partial a_1$, $\partial C_i^0 / \partial a_t$, $\partial C_i^0 / \partial \ln(k)$.
- [2] Solve for matrices from equations (A-43), (A-44) and (A-45).
- [3] Solve for column matrices from equations (A-41) and (A-42).
- [4] Solve for the mean and variance of $C_i^{t+\Delta t}$ from equations (A-49) and (A-50).

These computations combine the FOSM method and finite elements and have been implemented using FORTRAN.

The two examples shown below present and compare the numerical results using both

FOSM method and Monte Carlo simulations. Moreover, in order to verify the method using an analytical solution, a line source is placed on one end of the study field to emulate an one-dimensional problem as in case one (Table A-3):

Table A-3. Input Data for the Case 1.

Initial pollutant concentration (mg/l)	2.0
The magnitude of hydraulic gradient	0.1
The contaminant release time(day)	500
The down-gradient of the source(m)	10
Desired number of Monte Carlo simulations	200
Mean and standard deviation of log-conductivity(m/day)	-3, 0.5
Mean and standard deviation of dispersivity	60, 10

Table A-4. Comparison of Finite Elements and Monte Carlo Simulations for Case 2.

<i>Analytical solution</i>	<i>mean value</i>	<i>standard deviation</i>	<i>COV</i>
FOSM method	1.21903	0.210508	0.172685
Monte Carlo simulation	1.21992	0.228937	0.187666
<i>Finite element solution</i>			
FOSM method	1.26367	0.187178	0.148125
Monte Carlo simulation	1.27021	0.195496	0.153908

The results presented in Table A-4 above show good agreement between the FOSM method and Monte Carlo simulations, for both the analytical solutions and finite element solutions. For the second case, smaller values of mean and variance of hydraulic conductivity and dispersivity are used (see Table A-5). The results are presented in Table A-6: showing that the differences between the mean contaminant concentration values among these four different approaches are very small (less than 1 %). Also, there is much better agreement between the FOSM method and the Monte Carlo simulation for the case of finite element solutions.

Table A-5. Input Data for the Case 1.

Initial pollutant concentration (mg/l)	2.0
The magnitude of hydraulic gradient	0.1
The contaminant release time(day)	500
The down-gradient of the source(m)	10
Desired number of Monte Carlo simulations	200
Mean and standard deviation of log-conductivity(m/day)	0 , 0.1
Mean and standard deviation of dispersivity	10 , 1

Table A-6. Comparison of Finite Elements and Monte Carlo Simulations for Case 2.

<u>Analytical solution</u>	<u>mean value</u>	<u>standard deviation</u>	<u>COV</u>
FOSM method	1.95116	0.018463	0.009463
Monte Carlo simulation	1.95196	0.012023	0.006159
<u>Finite element solution</u>			
FOSM method	1.95144	0.011885	0.006090
Monte Carlo simulation	1.95227	0.011735	0.006011

3. Example three

For this example, a two-dimensional advection-dispersion transport for a heterogeneous medium in a uniform flow field is studied, two types of soils are specified and they are spatially correlated. For convenience, an index flag, $index(e)$ is used to record the type of soil at element (e) within the study site:

$$D_l(index(e)) = a_l(index(e)) \times v_x(index(e)) \quad (A-51)$$

$$v_x(index(e)) = k(index(e)) \times I \quad (A-52)$$

$$G_{li}^e = \int \int \{ D_l(index(e)) \left(\frac{\partial N_i^e}{\partial x} \frac{\partial N_l^e}{\partial x} + D_t(index(e)) \frac{\partial N_i^e}{\partial y} \frac{\partial N_l^e}{\partial y} \right) \} dx dy \quad (A-53)$$

$$U_{li}^e = v_x(index(e)) \int \int \frac{\partial N_i^e}{\partial x} N_l^e dx dy \quad (A-54)$$

$$\begin{aligned} \frac{\partial (G_{li}^e + U_{li}^e)}{\partial v_x(j)} = & \int \int \{ a_l(index(e)) \left(\frac{\partial N_i^e}{\partial x} \frac{\partial N_l^e}{\partial x} + a_t(index(e)) \frac{\partial N_i^e}{\partial y} \frac{\partial N_l^e}{\partial y} \right) \right. \\ & \left. + \frac{\partial N_i^e}{\partial x} N_l^e \right\} \delta(index(e), j) dx dy \end{aligned} \quad (A-55)$$

$$\frac{\partial G_{ij}}{\partial a_i(j)} = \int \int v_x(\text{idex}(e)) \frac{\partial N_i^e}{\partial x} \frac{\partial N_j^e}{\partial x} \delta(\text{idex}(e), j) dx dy \quad (\text{A-56})$$

$$\frac{\partial G_{ii}}{\partial a_i(j)} = \int \int v_x(\text{idex}(e)) \frac{\partial N_i^e}{\partial y} \frac{\partial N_i^e}{\partial y} \delta(\text{idex}(e), j) dx dy \quad (\text{A-57})$$

where $\delta(\text{idex}(e), j)$ is the Kronecker delta (i.e. $\delta(i, j) = 1$ if $i = j$, whereas $\delta(i, j) = 0$ if $i \neq j$).

Therefore, the resulting mean and variance of $C_i^{t, \Delta t}$ are

$$\mu(C_i^{t, \Delta t}) = C_i^{t, \Delta t}(\mu(\ln(k)), \mu(a_i), \mu(a_e)) \quad (\text{A-58})$$

$$\begin{aligned} \text{var}(C_i^{t, \Delta t}) &= \sum_{n=1}^2 \sum_{j=1}^2 \frac{\partial C_i^{t, \Delta t}}{\partial a_i(j)} \frac{\partial C_i^{t, \Delta t}}{\partial a_i(n)} \text{Cov}(a_i(j), a_i(n)) \\ &+ \sum_{n=1}^2 \sum_{j=1}^2 \frac{\partial C_i^{t, \Delta t}}{\partial a_e(j)} \frac{\partial C_i^{t, \Delta t}}{\partial a_e(n)} \text{Cov}(a_e(j), a_e(n)) \\ &+ \sum_{n=1}^2 \sum_{j=1}^2 v_x(j) v_x(n) \frac{\partial C_i^{t, \Delta t}}{\partial v_x(j)} \frac{\partial C_i^{t, \Delta t}}{\partial v_x(n)} \text{Cov}(\ln(k(j)), \ln(k(n))) \end{aligned} \quad (\text{A-59})$$

The numerical example shows satisfactory results from using the first-order method comparing to the one from 500 Monte Carlo simulations (Figure A-10). Note that the first order method only used 7 cpu time, while 500 Monte Carlo simulations utilized more than 80 cpu time.

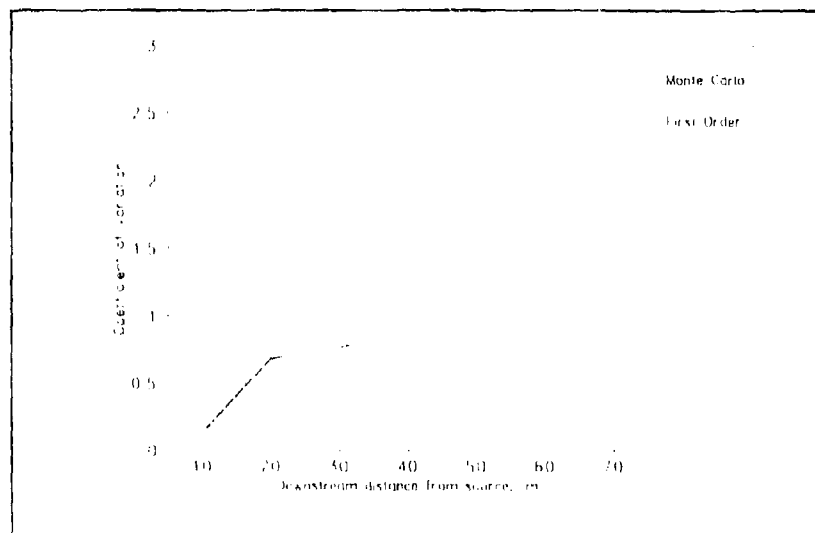


Figure A-10. The dispersion of variation of pollutant in a heterogeneous field with $\mu_{\ln(k_1)} = -3$, $\text{Var}_{\ln(k_1)} = 0.25$, $\mu_{\ln(k_2)} = -2.5$, $\text{Var}_{\ln(k_2)} = 0.1$, $\text{Cov}_{\ln(k_1), \ln(k_2)} = 0.04$, $\mu_{a_1} = 60$, $\text{Var}_{a_1} = 100$, $\mu_{a_2} = 70$, $\text{Var}_{a_2} = 120$, $\text{Cov}_{a_1, a_2} = 110$.

The results presented in this Appendix show that without requiring a full description of the probability distribution of model parameters, the FOSM method can still adequately estimate the mean and variance properties of contaminant concentration predictions in both homogeneous and heterogeneous random fields. The reliability analysis using FOSM method shows good agreement with Monte Carlo simulations in both analytical solutions and numerical (finite elements) method. The results illustrate that a significant tradeoff exists in the amount of computational effort required in determining the cumulative distribution of the contaminant concentration.